Complex Systems Science for Subsurface Fate and Transport

Report from the August 2009 workshop
Subsurface Biogeochemical Research (SBR)

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Biological and Environmental Research

1. Overview of SBR: Goals and Approach
2. Strategic Planning
3. Workshop – August, 2009
Biological and Environmental Research Mission

• To understand complex biological, climatic, and environmental systems across spatial and temporal scales.

• BER provides the foundational science to:
  – Support the development of next generation biofuels
  – Understand and predict the potential effects of greenhouse gas emissions on Earth’s climate and biosphere – the energy-climate nexus
  – **Understand and predict processes in subsurface environments**
  – Develop new tools to explore the interface of biological and physical sciences
Biological and Environmental Research Approach

- Understanding complex biological and environmental systems across many spatial and temporal scales:
  - From the sub-micron to the global
  - From individual molecules to ecosystems
  - From nanoseconds to millennia

- **Integrating science by tightly coupling theory, observations, experiments, models, and simulations**

- Supporting interdisciplinary research to address critical national needs

- Engaging national laboratories, universities, and the private sector to generate the best possible science
Subsurface Biogeochemical Research (FY10 - $50M)

• Advancing a fundamental understanding of coupled physical, chemical, and biological processes controlling contaminant mobility in the environment
  – Addressing DOE issues in intractable environmental remediation, long-term site stewardship, and nuclear waste disposal
  – Current contaminants of concern: U, Tc, Pu, ⁹⁰Sr, ¹³⁷Cs, ²³⁷Np, Hg, Cr, I
Subsurface Research Across Scales

Integrative, multidisciplinary approaches to understanding multi-scale processes controlling contaminant mobility in the environment.

- **Characterization and monitoring**
- **Microbiology, geochemistry, hydrology**
- **Modeling and high-performance computing**
- **Molecular science, EMSL, light sources**

- **Field scale** >10^3 m
- **Mesoscale** 10^{1.5}–10^3 m
- **Pore scale** 10^{-3}–10^{1.5} m
- **Microscopic** 10^{-7}–10^{-3} m
- **Molecular/nano** 10^{-10}–10^{-8} m
Iterative Environmental Microbiology

SBR Microbiology seeks a mechanistic and predictive understanding of microbial metabolism in the environment. Goal is to integrate subsurface microbial activity/growth with reactive transport models.
SBR Structure

Field Scale Research

Small(er) and fundamental scales

Increasing Complexity & Increasing Field Relevance

Computational Modeling & Iterative Experimentation

Predictive Understanding

Oak Ridge Y-12

Hanford 300 Area

Rifle UMTRA site

ORNL

PNNL

LBNL

ANL

SLAC

INL

LLNL

Universities

Academic Research

Lab SFAs
• Conduct workshop to identify knowledge gaps and science challenges that must be met to predict contaminant behavior in complex subsurface systems

• Using the logic model format, develop a strategic plan for the BER contaminant fate and transport research program for a ten year planning horizon

  • Evaluate utilization of existing program elements and resources, consider needs

  • Consider points of integration with other BER mission areas and leveraging of other DOE research programs and facilities

  • Consider overarching BER complex systems science philosophy
# The Logic of Logic Models

## Contaminant Fate and Transport

<table>
<thead>
<tr>
<th>Current Situation</th>
<th>Inputs / Resources</th>
<th>Near Term Goals (1-5 years)</th>
<th>Mid Term Goals (5-10 years)</th>
<th>Long Term Goals (10-15 years)</th>
<th>Outcomes (Impacts on science and society)</th>
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<tbody>
<tr>
<td>Inadequate understanding of the key biogeochemical and hydrodynamic processes which control contaminant fate and transport in the environment</td>
<td>Integrated SFA research programs</td>
<td>Goal 1</td>
<td>Goal 1</td>
<td>Goal 1</td>
<td>Improved understanding of contaminant transport and transformation through iterative, and interdisciplinary, experimentation and modeling.</td>
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<td>Linear engineering approach does not account for the inherent complexity of real earth systems which leads to ineffective approaches to site characterization, modeling and management/stewardship</td>
<td>Engaged university research community with multidisciplinary capabilities</td>
<td>Goal 2</td>
<td>Goal 2</td>
<td>Goal 2</td>
<td>Improved management of the impacts of environmental contamination from past nuclear weapons production and the long-term stewardship of nuclear waste</td>
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<td>Integrated Field Research Challenge (IFRC) sites</td>
<td>Goal 3</td>
<td>Goal 3</td>
<td>Goal 3</td>
<td>Reduced risks to human health and the environment.</td>
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<td>EMSL, JGI, SciDAC, BES Geosciences, BES User Facilities</td>
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<td>EM, LM, USGS</td>
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Desired Outcomes

* Reduce risk to human health and the environment;
* Reduce costs for cleanup and stewardship;
* Increase reliability and public acceptance

- Improved approaches to understand and predict model contaminant fate and transport in realistically complex environments

- Improved approaches to assess and control the long-term stability of contaminants at DOE sites
DOE-BER Workshop

Complex System Science for Subsurface Fate and Transport

Workshop Co-Chairs
Frank Loeffler  John Zachara  Susan Hubbard
Workshop Goal and Objectives

**Goal** – *Identify knowledge gaps and science challenges that must be met to predict contaminant behavior in complex subsurface systems*

**Objectives:**

- *Define complex subsurface systems* and establish why they are important to different DOE environmental and energy mission outcomes
- Consider how the *coupling of subsurface processes* (hydrological, microbiological, and geochemical) defines complex system response and dynamics
- Evaluate *research approaches* that can be used to identify and account for the influence of smaller scale processes and their mechanisms on larger scale system behavior.
- Conceptualize models needed to describe and *predict complex system behavior* at different scales.
- Identify significant, long-term, *interdisciplinary research opportunities* associated with complex subsurface systems.
There are no universal laws

There is not even a universally accepted definition for “complex system science” or for what makes a system “complex”

But, there are similar characteristics and attributes: emergent phenomena, intermittency, coupling across scales, ... (climate, ecosystems, microbial systems, ...)

And, perhaps, similar research approaches can be developed, or adapted from one system to another => to advance our predictive understanding of complex system behavior

“Each complex system is different; apparently there are no general laws for complexity. Instead, one must reach for “lessons” that might, with insight and understanding, be learned in one system and applied to another” - Goldenfeld and Kadanoff (Dan Rothman)
Complex System Science vs. Systems Biology

- **Complexity methods** often use
  - A top-down approach to identify key interactions controlling diagnostic variables at the prediction scale;
  - General macroscopic laws controlling system-scale behavior;
  - Simplified models of subsystem interactions that enable prediction

- This approach is **analogous to systems biology**, which is defined, in the context of Biological Systems Science research programs in BER as
  - “the holistic, multidisciplinary study of complex interactions that specify the function of an entire biological system—whether single cells or a multicellular organism—rather than the reductionist study of individual components.”

- Both approaches emphasize the tight coupling between experimentation, observation and modeling
Overview of Workshop Structure

**When**
- Monday Afternoon & Evening
- Tuesday Morning & Early Afternoon
- Tuesday Late Afternoon/Evening and Wednesday Morning

**Products**
- Descriptions of Key Complex Systems & Attributes
- Logic Model: Discipline-Based Research Goals
- Logic Model: Integrated Complex Subsurface System Research Goals

**Breakout #1:**
Identify Favorite Complex Systems *by Scale*

**Breakout #2:**
Identify Key Research Priorities for Investigating Complex Subsystems *by Discipline*

**Breakout #3:**
Define Complex Subsurface System Challenges and Research Goals *across Scales and Disciplines*
# Workshop Discussion

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<th>Reductionism</th>
<th>Complexity</th>
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| **Philosophy** | Overall system behavior can be understood from a detailed understanding of the system components | “More is Different” => Emergence  
Seek to indentify and understand commonalities between complex systems and their relationship to more simple systems |
| **Strategy**  | Understand and model system behavior as some permutation of the sum of its lower scale parts – blame heterogeneity for shortcomings | Identify diagnostic variables and transferable macro-scale laws that define/describe high-level system behavior |
| **Research Approach** | Bottom-Up: mechanistic | Top-Down: phenomenological |
| **Modeling** | Mechanistic details of lower scale processes are preserved but streamlined in upscaling. Models are “calibrated” to account for the effects of heterogeneities | Phenomenological models are used to explain and describe key processes contributions, interactions, and properties that control system behavior |
Hybrid Approach: Reductionism + Complexity

- A pragmatic melding of bottom-up and top-down approaches.
- Emphasize the identification and understanding of key underlying mechanisms and interactions, and the importance of scale transitions, while simultaneously providing insights on common macroscopic laws governing complex system behavior at the prediction scale.
- Goal is to achieve comprehensive and quantitative system predictability through iterative experimentation and modeling.
## Complex System Research Opportunities

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<tr>
<th>Research Opportunity</th>
<th>Challenge</th>
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<tr>
<td></td>
<td>Microbial Community Responses in Dynamic Subsurface Conditions</td>
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<td>Biogeochemical Rates in Heterogeneous Media</td>
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<td>Feedbacks Between Biogeochemical Transformations and Flow</td>
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<tr>
<td>2. Identify and Quantify Scale Transitions in Hierarchical Subsurface Systems</td>
<td>Measurement Approaches for Key Variables and Diagnostic Signatures</td>
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<td>Identification of Smaller-Scale Controlling Variables</td>
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<td>Scale Transition Models</td>
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<td>3. Understand Integrated Subsurface System Behavior</td>
<td>Identification of Field-Scale Emergent Phenomena</td>
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<td>Strategies for Interrogating Large-Scale Behavior</td>
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<td>Phenomenological Models for Prediction</td>
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Summary and Workshop Findings

- **Apply a hybrid research approach** to advance predictive understanding of hierarchical subsurface systems by combining complimentary bottom-up reductionism with top-down complexity concepts through *iterative experimentation and modeling*.

- Focus well-conceived, hybrid research efforts at selected **DOE-relevant field study sites, and representative laboratory model systems** at different scales, that offer the most potential for understanding fundamental process interactions that occur across scales and lead to complex subsurface behavior.

- Explore the value of complex system science approaches in providing the scientific basis for effective DOE management of earth/environmental systems.
Without investment and leveraging

SC = $50M/$20M/$2M

$9M ASCEM $6M Core

$Billions

Scientific Opportunities to Reduce Remediation Risk: Translating Fundamental Science into Cost-saving Applied Solutions

EM site cleanup and closure

$Billions

Cleanup costs

Without investment and leveraging

With investment and leveraging

Time

Environmental Management

safety  performance  cleanup  closure
Thank you!