

# Proposed

# LBNL Subsurface Science SFA



- Motivation & Critical Challenges
- SFA Structure
- Scientific Research Areas
  - Area 1 Sustainable Systems Biogeochemistry
  - Area 2 Integrated Characterization, Modeling and Monitoring
- Field Study Sites
- Collaborators & Facilities

Susan Hubbard (sshubbard@lbl.gov)
Presented on behalf of LBNL SFA Research Team



# **Motivation**

The production and testing of nuclear weapons has created a vast volume of subsurface legacy contamination that the DOE has the responsibility to locate, clean up, and monitor.

DOE spends \$6B/year and is expected to spend approximately \$200B through 2070 on cleanup efforts



A **predictive understanding** of multi-scale, coupled, in-situ processes and technological developments could improve and reduce the enormous cost associated with legacy waste clean up

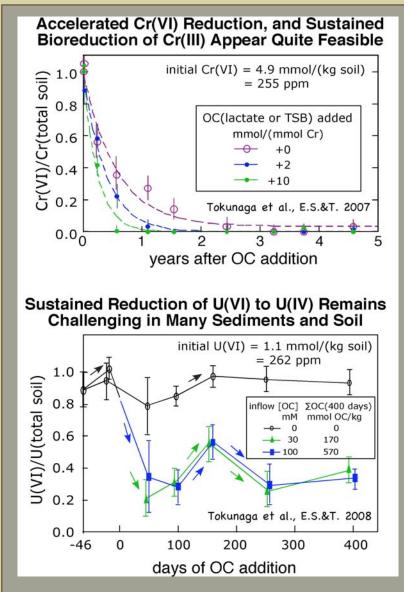
# Sustainable Systems Biogeochemistry: Critical Challenge



- Metals and many radionuclides pose daunting remediation challenges because they do not degrade to benign products, or only do so through very slow radioactive decay
  - Half-life of <sup>238</sup>U is 4.5 billion years
  - Half-life of <sup>90</sup>Sr is 29 years

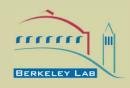
Sciences

- Contaminated regions will be exposed to ambient biogeochemical conditions once remedial treatments have ceased.
- A critical challenge is to develop remediation strategies for metals and radionuclides that are compatible with prevailing hydrobiogeochemical conditions so that the treatment will be sustainable.



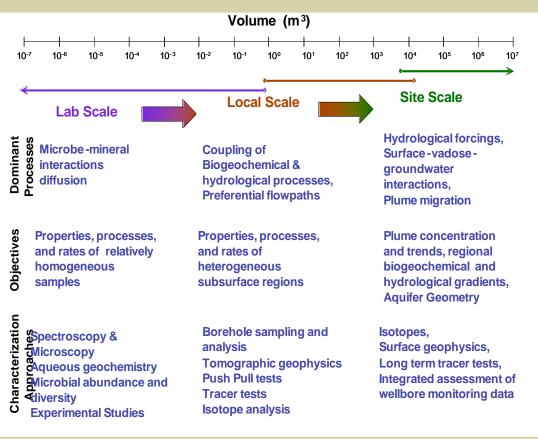


# Characterization and Modeling: Critical Challenge



The natural variability, scale-dependence, and coupled nature of subsurface hydrobiogeochemical properties renders characterization and mechanistic reactive transport modeling challenging.

This obstacle in turn often leads to our inability to successfully implement field-scale remediation strategies.



Looney&Hubbard, 2006

A critical challenge is to develop capabilities to quantify and predict subsurface processes in natural systems and over fieldrelevant scales



# LBNL Subsurface Science SFA





# **CHARACTERIS**TICS

ddresses critical challenges in subsurface environmental science;

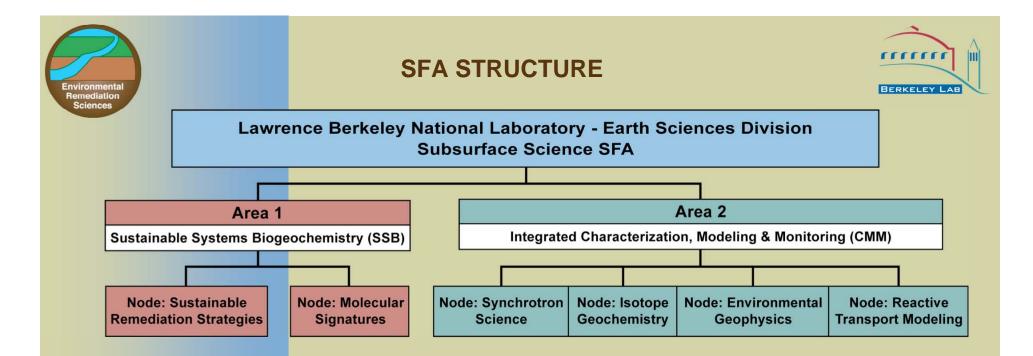
tilizes our recognized expertise and facilitates but permits growth in needed areas;

ncourages team-based as well as individual science contributions;

as significant potential for impact to DOE cleanup/stewardship

ligned with and leverages on collaborative efforts;

s flexible to permit investigation in new directions while maintaining ERSP SFA Review April 9, 2008

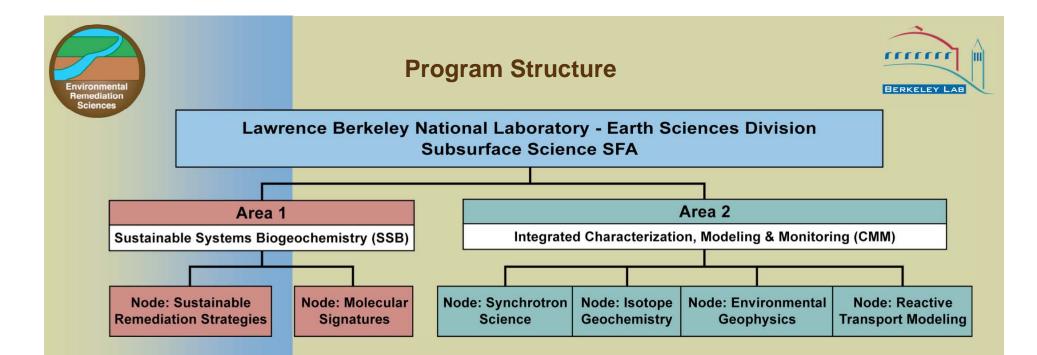


#### The SFA is hierarchically structured:

 Scientific Research Areas create synergy between scientists working on two critical challenges;

• The **Nodes** create synergy within smaller groups of scientists performing theme- or approach-based research, and to serve as a nucleus for collaborations;

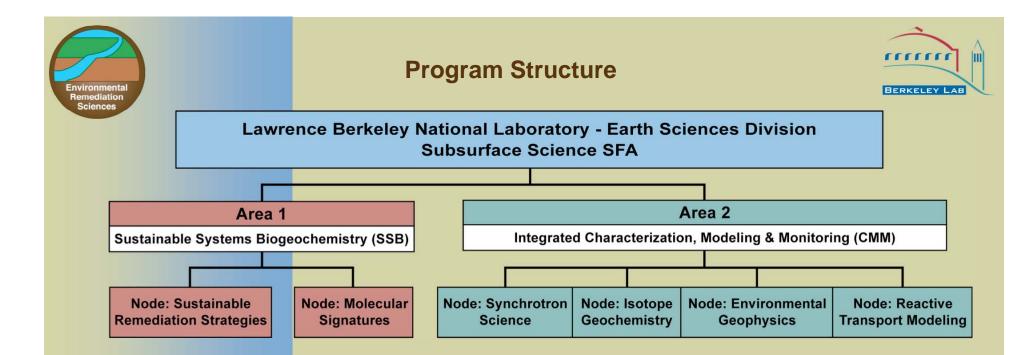
• **Projects** address Node objectives and contribute to goal of Scientific Research Areas.



#### Area 1 Critical Challenge:

Improve and quantify understanding of biogeochemical processes needed to design scientifically defensible and *sustainable* remediation strategies

Two theme-based Nodes



#### Area 1 Critical Challenge:

Improve and quantify understanding of biogeochemical processes needed to design scientifically defensible and *sustainable* remediation strategies

#### Area 2 Critical Challenge:

Develop an unprecedented ability to quantify and predict subsurface processes associated with natural attenuation and active remediation through improvements in and coupling between characterization, modeling, and monitoring.

Two theme-based Nodes

Four approach-based Nodes.



#### **Field Study Sites**

Explore enhanced sustainability of Cr(VI) bioremediation at the Hanford 100 Area

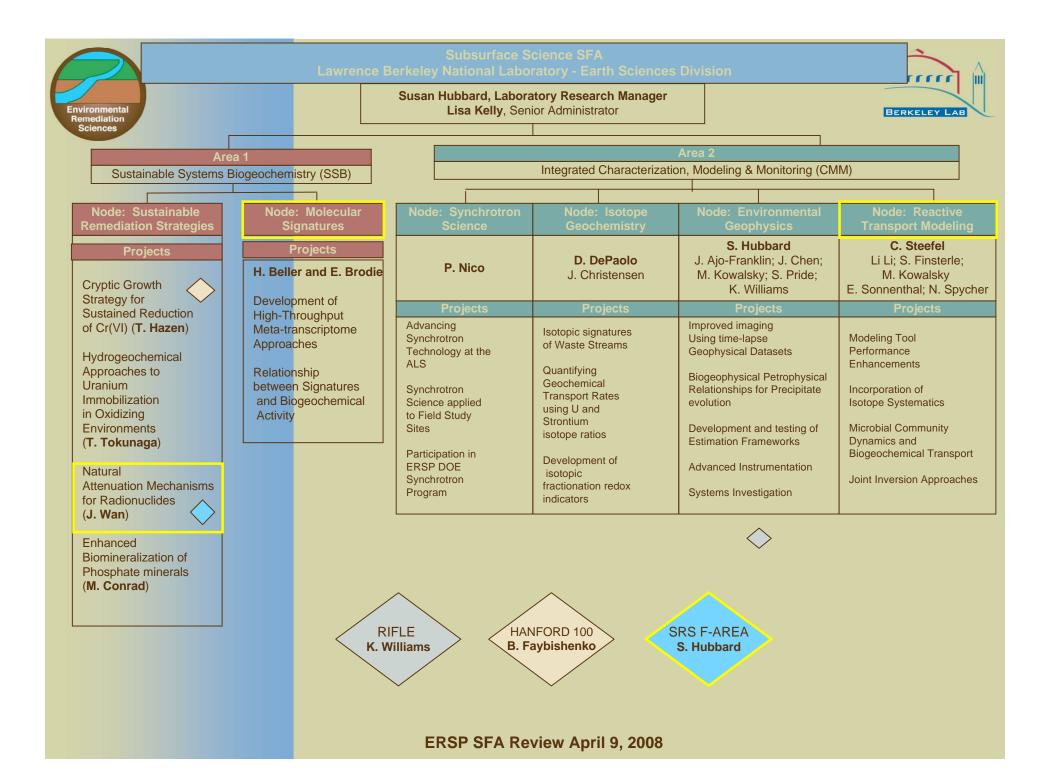


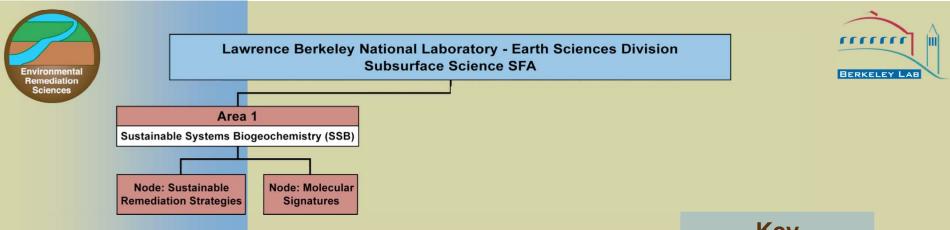


Develop a scientific basis for monitored natural attenuation of <sup>90</sup>Sr, <sup>129</sup>I and U at the **Savannah River Site F-Area.** 

Integration of multiple CMM approaches to explore feedbacks between flow and transformations at the U contaminated Rifle IFC







### **Two Theme-Based Nodes in Area 1 SSB:**

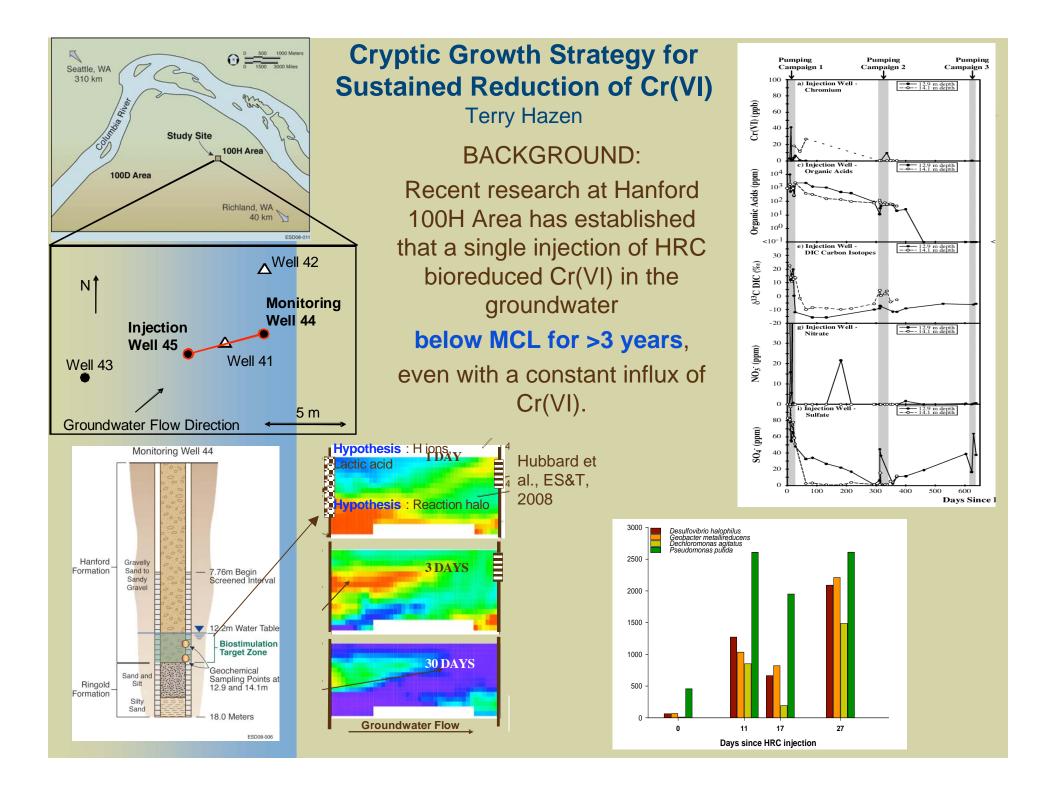
- The Sustainable Remediation Strategies
   Node will focus on understanding processes
   and on developing specific approaches relevant
   to sustainable engineered remediation and
   natural attenuation of key contaminants.
- The Molecular Signatures Node will facilitate discovery of genes that are associated with bioremediation-relevant microbial activities.

Key Investigators \*Harry Beller \*Eoin Brodie Mark Conrad Mark Conrad Terry Hazen Tetsu Tokunaga Jiamin Wan



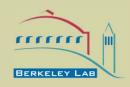


- Sustainable remediation of subsurface Cr, U, <sup>90</sup>Sr, and <sup>129</sup>I contaminated systems.
- Four key projects expected synergistic exchanges:
  - Remediation of U-contamination will be investigated under a range of conditions in three projects.
  - Redox coupling of NO<sub>3</sub><sup>-</sup>, Mn and Fe to U and Cr contaminants will be explored in two projects.
  - Contaminant stabilization under oxidizing conditions is a theme common to two projects.
- Some of the fundamental studies conducted in the SSB Area will be:
  - Carried out concurrently with studies in Area 2;
  - Implemented at the Field Study Sites .





# Project: Cryptic Growth Strategy for Sustained Reduction of Cr(VI) Terry Hazen

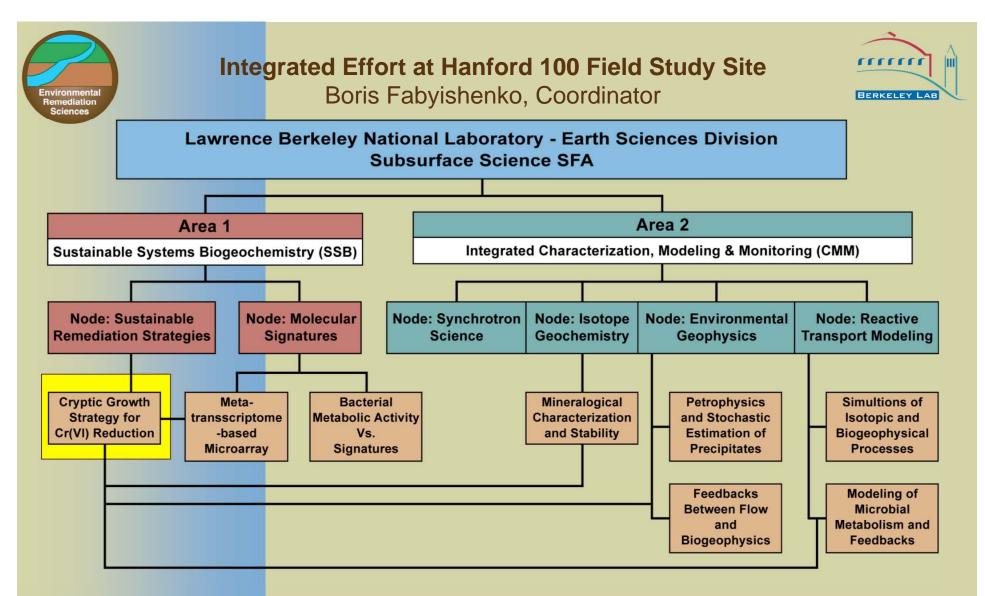


# **Project Objectives:**

- Explore the hypothesis that a cryptic growth mechanism is responsible for the sustained reduction, where:
  - Lysis of dead cells contribute to the substrate;
  - Recycling via cryptic growth promotes sustained reduction.
- Leverage with Genomics: GTL push pull testing to explore hypothesis that stressor resiliency can be caused by the formation of microbial assemblages that syntropically function over a wide range of redox conditions.



Project part of Hanford 100 Field Study Site.....



Reduction Mechanism (Direct enzymatic? Abiotic? A combination?) Mechanism and quantities of Cr(III) precipitates? Dependence of sustained bioreduction on in-situ microbial structure? Relevance of findings at 100H to 100D? Role of heterogeneity on sustained bioreduction?



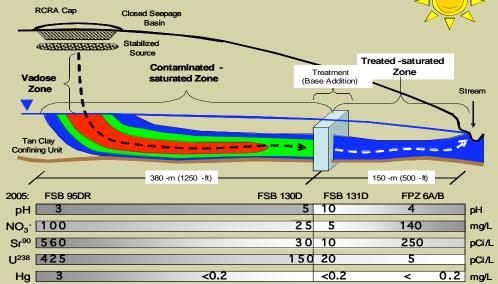
# Project: Natural Attenuation Mechanisms of Contaminant Radionuclides at the Savannah F-Area Jiamin Wan

### BACKGROUND

Savannah River Site F-Area acidic plume includes U, <sup>90</sup>Sr, <sup>129</sup>I, and <sup>99</sup>Tc;

DOE is planning to make the transition from the years of active remediation to monitored natural attenuation (MNA).

HYPOTHESIS. Sorption and desorption are the dominant processes controlling natural attenuation, and development of site-specific equilibrium/kinetic surface complexation model can be used to assess if MNA is a viable strategy for the F-Area



**APPROACH.** Laboratory experiments to measure sorption and desorption rates/extents for U, 90Sr, and 129I on acid-altered and the pristine sediments as a function of pH and facies, coupled with:

- •Synchrotron methods to determine contaminant speciation.
- •Isotopic analyses to track the fate, transport, and rates of contaminants
- •Reactive transport modeling



### Savannah River Site F-Area Field Study Site



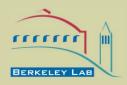




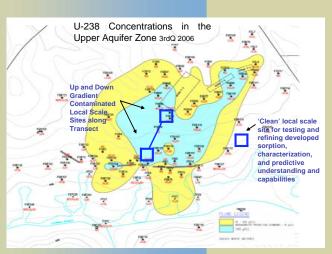
Discovery Research	Use -inspired Basic Rese	arch Appli	ed Research	Technology Maturation & Deployment
U.S. DEPART	Office of Science			ronmental Management performance & cleanup & closure
Goal: New know Focus: Phenom Metric: Knowled	nena		Goal: Practic Focus: Perfo Metric: Miles	
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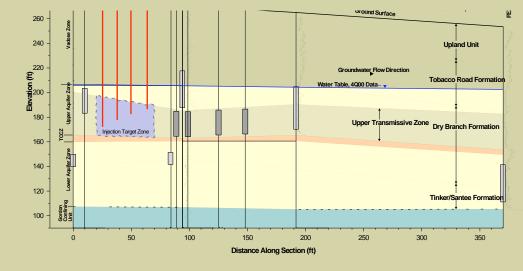


#### LBNL Foci at SRS F-Area Field Study Site



- Geochemical Process. Sorption models can be developed to quantify rates of key metal and radionuclide constituents as a function of pH and reactive facies.
- Characterization. Development and implementation of Isotopic Indicators and Reactive Facies Framework to facilitate the characterization of critical hydrobiogeochemical processes and rates across scales
- Reactive Transport Modeling. Through incorporation of developed faciesbased sorption model and facies-based multi-scale characterization, mechanistic reactive transport modeling of plume evolution and migration can be performed with sufficient accuracy to predict behavior of system over field relevant scales



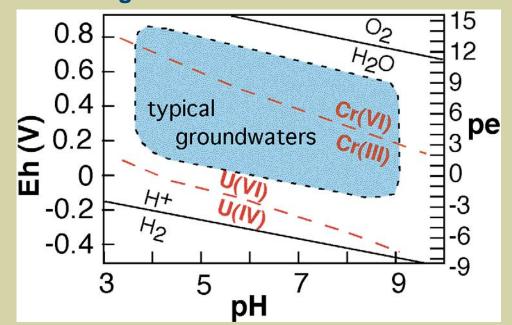




### Project: Hydrogeochemical Approaches to Uranium Immobilization in Oxidizing Environments Tetsu Tokunaga



- U contaminated environments are not naturally strongly reducing.
- Sustaining U bior require indefinite electron donor.
- **Objective:** Identify strategies for sustainable remediation of Ucontaminated systems that are compatible with prevailing oxidizing site conditions.



Sustainability of an in-situ redox manipulation can be partly evaluated by comparing the targeted redox state with redox conditions that prevail in the subsurface.

#### Approach:

- 1. Re-evaluate all factors that can constrain groundwater U concentrations under oxidizing conditions and select candidate strategies.
- 2. Batch testing of U(VI) removal from aqueous phases of contaminated sediments, combined with XRD and EXAFS for determination of resulting solid and surface U(VI) phases.
- 3. Laboratory column testing of U(VI) immobilization strategies
- 4. Field trial(s) of oxic-immobilization strategies.



### Project: Enhanced Vadose Zone Mineralization Mark Conrad



#### **MOTIVATION**

- Significant inventories of vadose zone contaminants pose a long-term threat to groundwater at a number of DOE sites.
- Phosphates are stable under oxic conditions and will readily incorporate <sup>90</sup>Sr and U into their mineral structure and will scavenge them from coexisting pore fluids.

# OBJECTIVE. Develop strategies to promote precipitation of phosphate minerals in unsaturated rocks and sediments.

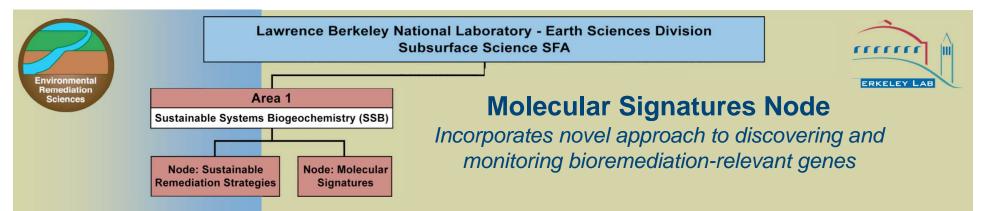
•Tri-ethyl phosphate (TEP) is an organophosphate compound that may provide good phosphate source for mineralization and can be readily distributed in unsaturated materials.

# **APPROACH.** Using experimental and numerical approaches:

Identify mineral precipitates and reaction rates;
Quantify U and <sup>90</sup>Sr uptake.

•Develop strategies for enhancing microbial rates of TEP degradation and phosphate release under variably saturated conditions.





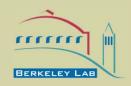
# **MOTIVATION**

The vast metabolic and phylogenetic diversity in natural subsurface systems poses a challenge, as all key gene/protein sequences needed to monitor bioremediationrelevant activities are not available in data repositories (e.g., GenBank).

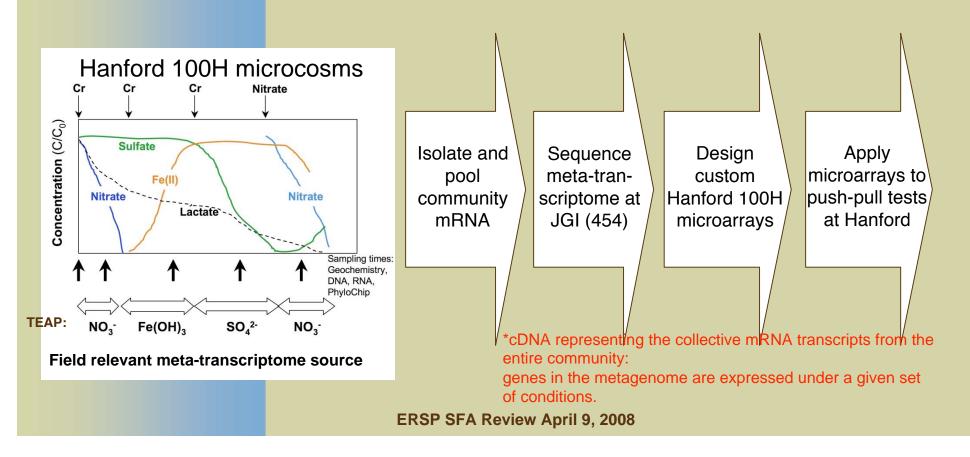
Need to integrate molecular-level understanding to specific, bioremediation-relevant metabolic activities simulated in reactive transport modeling.



# Molecular Signatures Node Harry Beller and Eoin Brodie



**OBJECTIVE (meta-transcriptome-based microarrays)**: Develop a novel and highthroughput approach that uses the meta-transcriptome\* to design high density oligonucleotide microarrays that can be used to identify highly expressed genes in a specific community under conditions of interest, without requiring any *a priori* hypotheses about which genes the community might be expressing or prior sequence information from data repositories. Bioremediation-relevant Signature Discovery

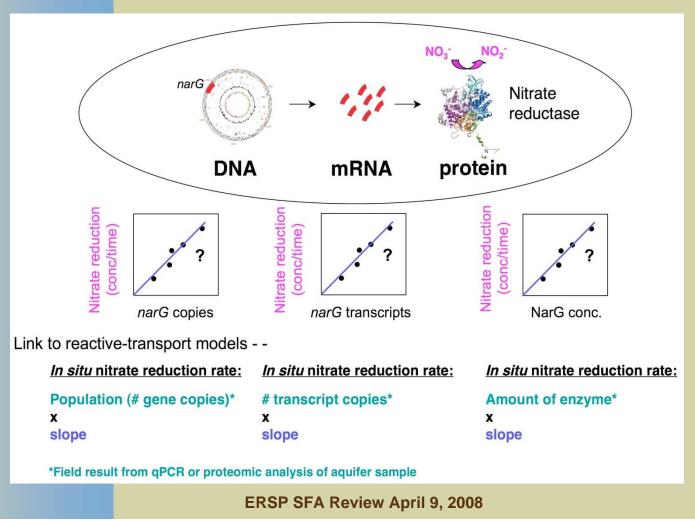


# Molecular Signatures Node Harry Beller and Eoin Brodie

Environmenta Remediation Sciences



**OBJECTIVE:** 'Activity signature correlations': Use well-characterized bacterial cultures to assess whether correlations between biogeochemical activities and *field-measurable* molecular signatures (based on DNA, mRNA, or protein) exist. Eventual link with Reactive Transport Models

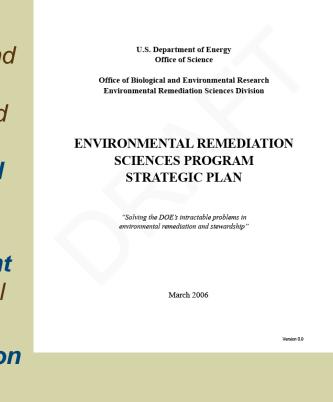




# The Sustainable Systems Biogeochemistry Area will address several ERSP Strategic Goals, including:



- "Determine key reactions and degradation pathways involved in radionuclide and metal transformations and immobilization";
- "Build on new tools in genomics and proteomics to explore the genetic diversity and dynamics of microbial communities (with an emphasis on how these communities respond to the stress of contamination and remediation, and how they can be sustained for the purposes of natural attenuation)";
- "Define and exploit microbial metabolic processes critical to controlling contaminant mobility" (using both remediation and natural attenuation)."
- "Develop sound foundations for remediation to guide decisions at DOE sites."





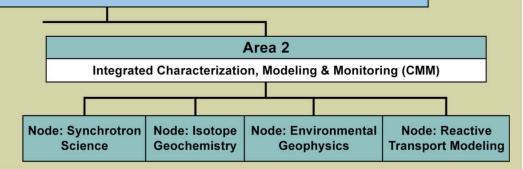
# Area 2



Lawrence Berkeley National Laboratory - Earth Sciences Division Subsurface Science SFA

# **Key Investigators**

\*Jonathan Ajo-Franklin Jinsong Chen John Christiansen Don DePaolo \*Stefan Finsterle Susan Hubbard \*Mike Kowalsky Peter Nico \*Steve Pride Eric Sonnenthal \*Nic Spycher Carl Steefel Ken Williams



OBJECTIVE: Develop an unprecedented ability to quantify and predict subsurface processes associated with natural attenuation and targeted manipulations.

#### •Four Approach-based Nodes

- •Projects will tackle challenges unique to each approach;
- •Document the synergies that come from integration of multiple approaches;
- •Test and implement advances at several Field Study Sites.



# **MOTIVATION:**

#### Synchrotron Science Node Peter Nico

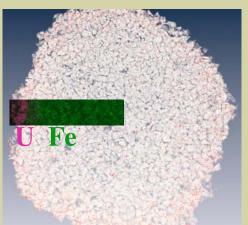


- Understanding of contaminant dynamics requires information about chemical form and distribution and associations in multiple dimensions.
- The Environmental suite of beamlines at the ALS span an energy range from infrared to hard x-ray, and spatial scales from nanometer to centimeter.

**OBJECTIVE:** Develop and apply new synchrotron techniques to interrogate physicochemcial properties and processes.

#### **APPROACH**

- Advance Environmental Synchrotron Technology at the ALS.
  - Integrated 3-D microtomography and 2-D microprobe chemical speciation.
  - Dynamic 3-D chemical and oxidation state imaging.
  - sFTIR for real time imaging of biomineralization processes.
- Integrate Synchrotron Science at Field Study Sites.



3D image of Fe coated sand aggregate with 2D image showing extent of U penetration after 20days

(Celine Pallud, Scott Fendorf)



Flow through 3-D microtomography chamber

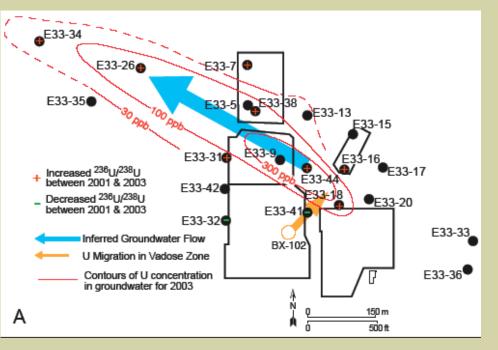


# Isotope Geochemistry Node Don DePaolo and John Christensen



**OBJECTIVE:** Improve the use of isotope measurements for developing conceptual models for and monitoring subsurface properties and processes.

> Tracking source and pathway of U contamination through vadose and groundwater at Hanford 200E Area (Christensen et al., 2004)



#### **MOTIVATION:** Provide constraints on:

- 1. Contaminant sources and fates;
- 2. Contaminant transport through the vadose zone and within groundwater;
- 3. Water-rock interaction, its mechanism and rates;
- 4. The extent, progress and mechanisms of biogeochemical transformation of contaminants



# Isotope Geochemistry Node Don DePaolo and John Christensen



# **APPROACH**

#### Isotopic Indicators of Redox Zonation.

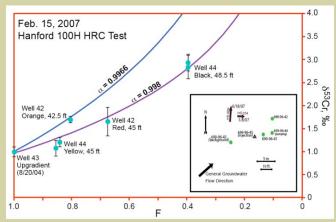
Laboratory experiments to determine isotopic fractionation factors for nitrate,  $CO_2$ , sulfate, Fe, Cr, and methane under various conditions and their changes during evolving conditions

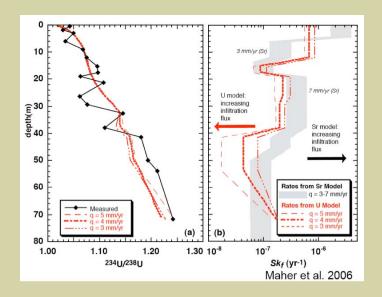
#### **Mineral/Fluid Interactions.**

Laboratory experiments to explore biogeochemical factors affecting Sr, Ca, Mg & U exchange between fluids and solids.

#### Synergies:

- Isotopic systematics into reactive transport models (w/RTM Node)
- Integration at Field Study Sites and other sites.





# Environmental Geophysics Node Susan Hubbard

#### 'Hydrogeophysics'

# **OBJECTIVE:**

Improve the use of geophysical methods for characterizing properties and monitoring processes associated with natural attenuation and active remediation.

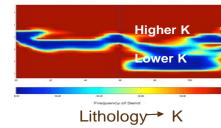
### **MOTIVATION:**

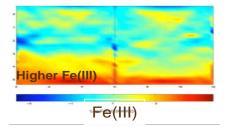
'Plume scale' characterization of flow properties;

Relationship between microscale processes and macroscale geophysical measurements;

Quantitative monitoring of biogeochemical transformations;

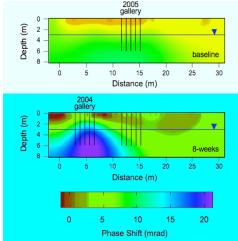
System process understanding.





Lithofacies and sediment geochemistry estimating (Chen et al., 2006)

#### 'Biogeophysics'



Development of an electrical phase anomaly associated with a biostimulation experiment (Williams et al., 2008)

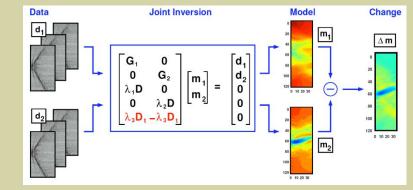
### Environmental Geophysics Node Susan Hubbard

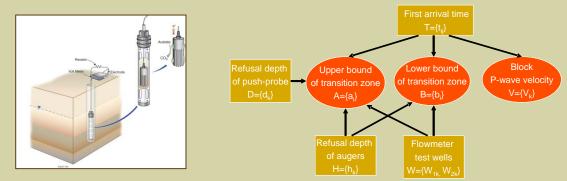
# **APPROACH**

Environmenta Remediation

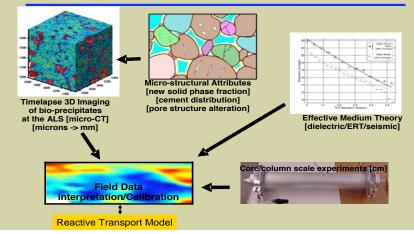
Sciences

- Imaging. Improve acquisition and inversion of time-lapse datsets;
- Petrophysics. Focus on geophysical responses to formation of precipitates and scaling;
- Estimation. Geochemical estimation framework and multi-scale reactive facies framework.
- Advanced Instrumentation.
   Electrode based approaches
   and continuous active source
   seismic system.
- Systems Investigations using above advances to explore feedbacks between flow characteristics and biogeochemical transformations.





Connecting Biologically-Induced Microstructures To Macroscopic (Geophysical) Properties





# Reactive Transport Modeling (RTM) Node Carl Steefel



# OBJECTIVE

 Develop capabilities to predict multi-scale, coupled, *in-situ* processes that govern sustained remediation or MNA of metals and radionuclides.

# MOTIVATION

- Efficient design and testing of remediation strategies
- Scientifically defensible predictions of natural attenuation
- Maximum use of fundamental science through development and application of "mechanistic" process models
- Multi-scale, multi-physics, multi-dimensional environmental problems require high performance computing



# **Reactive Transport Modeling Node Carl Steefel**

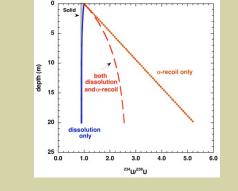


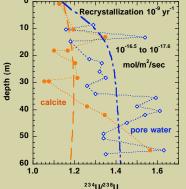
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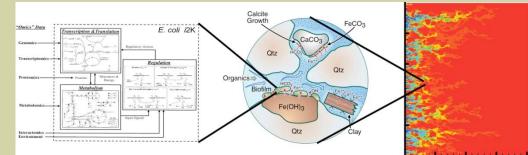
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# **APPROACH**

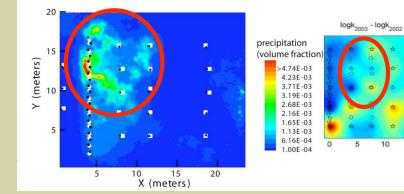
- Incorporation of stable and radiogenic isotopes into multicomponent RT models
- Coupling of microbial community dynamics and biogeochemical transport
- Joint geophysical-biogeochemical inversion approach

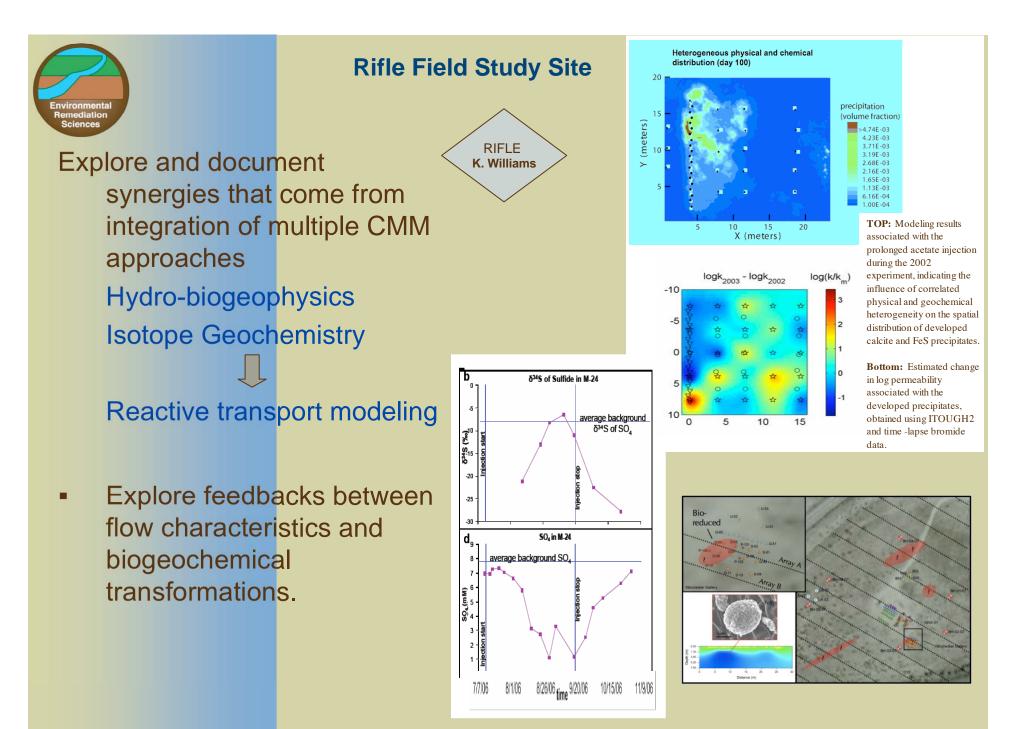






Enhancement of computational efficiency of Berkeley Lab RTM simulators



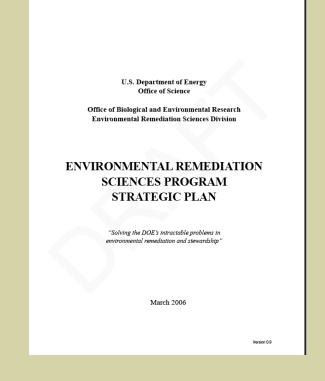


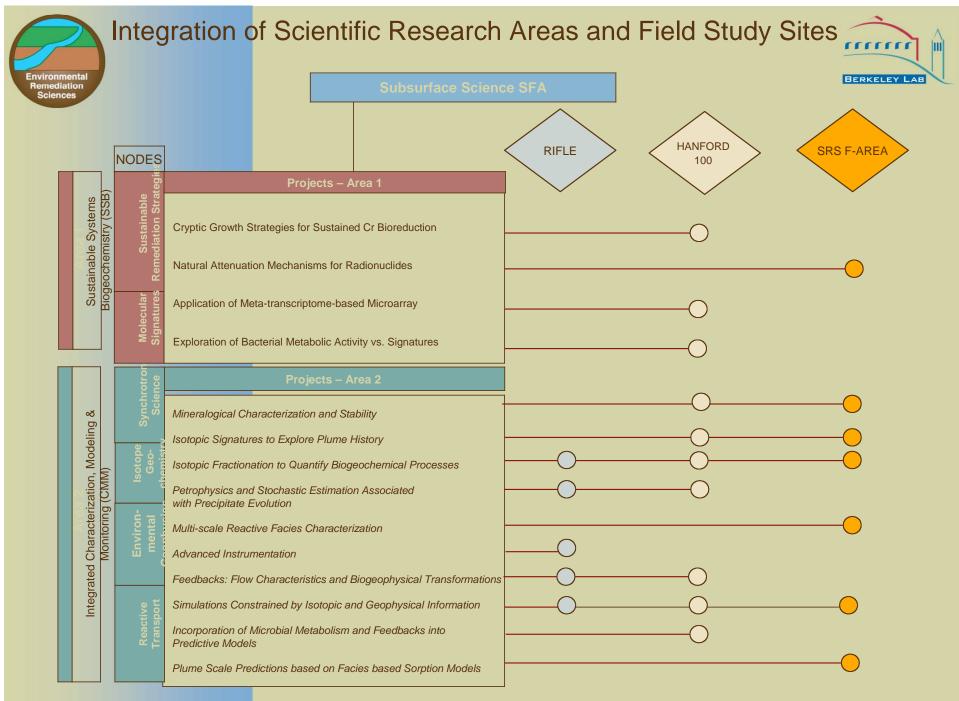




The Integrated Characterization, Modeling, and Monitoring Scientific Research Area will address several ERSP Strategic Goals, including:

- "Development of new measurement and monitoring tools that will permit interrogation of coupled biological, chemical, and physical processes in natural systems and often in a minimally invasive manner";
- "Improved ability to predict transport, transformations, and attenuation associated with remedial strategies";
- "Development of field-validated, robust tools for validation of predictive models and remediation strategies and for long-term performance modeling and of large-scale, fully coupled transport simulators".

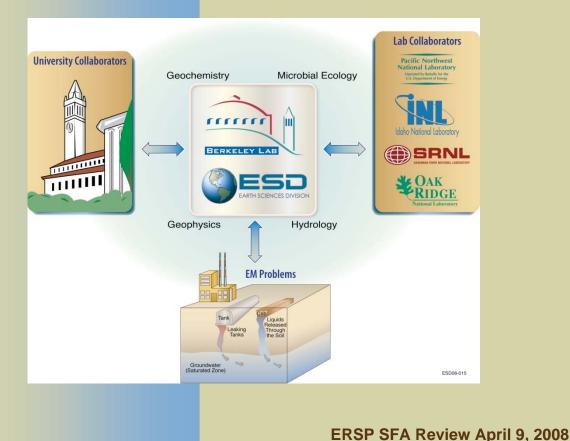


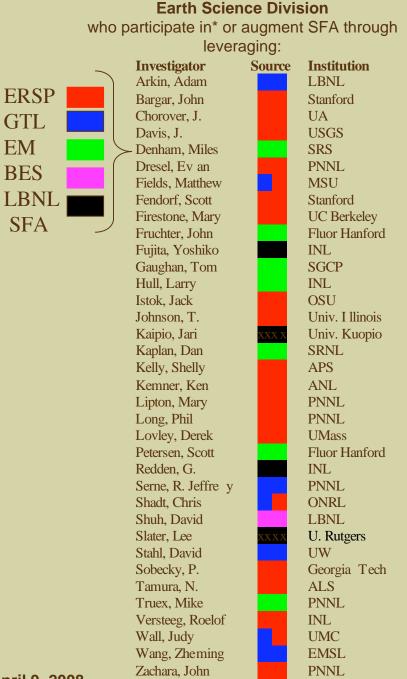




#### **LBNL SFA Collaborators**

The node structure has been designed to enhance existing and encourage new collaborations with University and National Laboratory Scientists, as well as increase the impact of ERSP science at EM sites.





Zhou, Jizhong

UO

COLLABORATORS to LBNL



# The program will take advantage of state-of-the-art *facilities* at LBNL.....

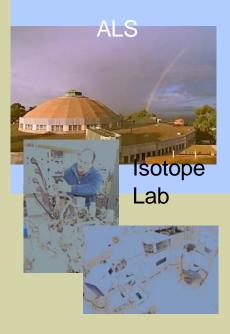


#### **Geophysical Computing**



**Molecular Foundry** 







Molecular Microbiology Lab





Rock and Soils Lab

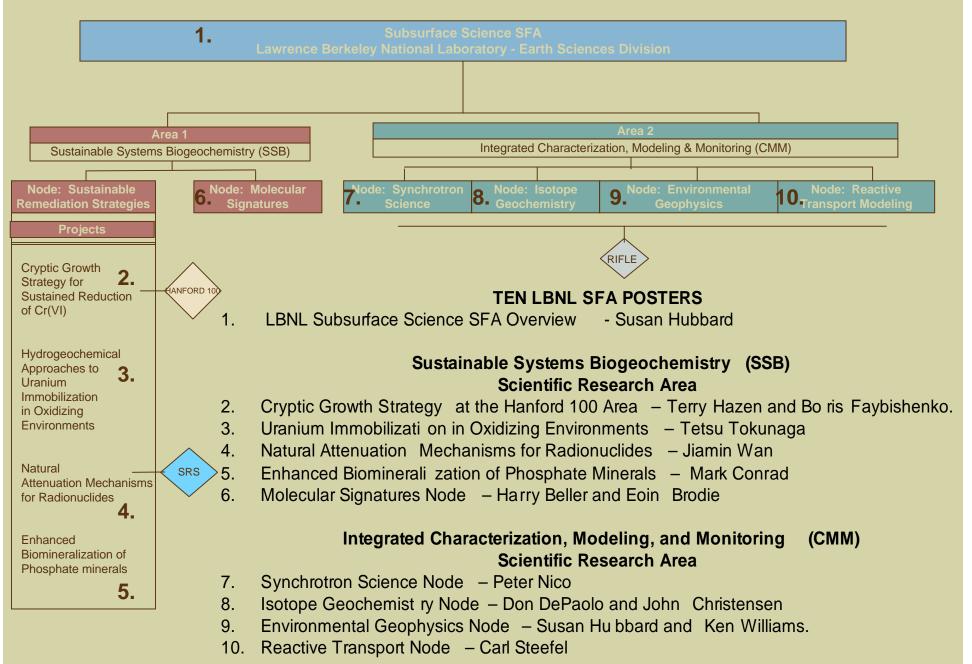


NERSC and Computing Cluster

#### .....as well as other ERSP-supported facilities.



# Thank you! Please visit our tern Posters:





# Summary



# The proposed SFA will:

- Address two critical environmental science challengesadvances should be relevant across the DOE complex;
- Utilize and extend LBNL's recognized capabilities and facilities;
- Promote synergy through multi-disciplinary and team-based research;
- Increase the impact of ERSP research to DOE clean-up effort.
- Thank you