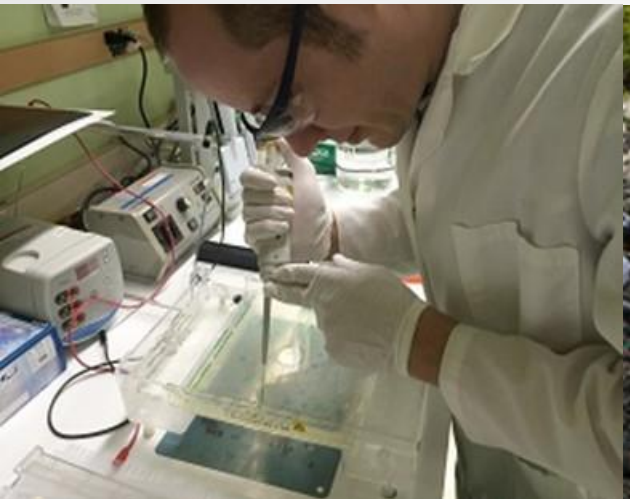


Complexity and Innovation: Advancing Watershed System Science

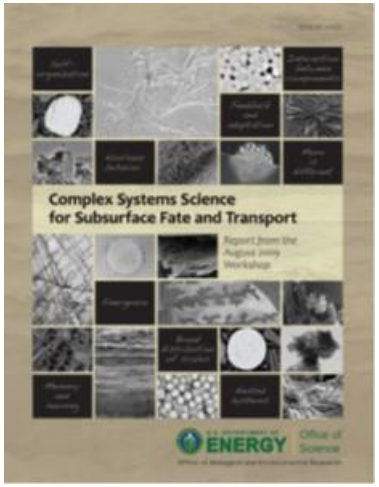
Tim Scheibe (PNNL), Susan Hubbard (LBNL)
& SBR Members

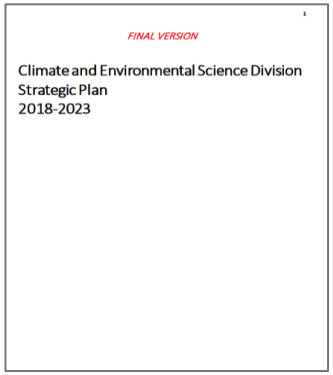
ESS PI Meeting
Potomac, MD, May 1-2, 2018



Past and Ongoing Visioning

SBR Complexity Workshop, 2010 → Many BER workshops 2011-2017 → SBR Visioning Meeting 2017 → **CESD Strategic Plan** 2018 → SBR Visioning Meeting Report 2018




FINAL VERSION

Climate and Environmental Science Division
Strategic Plan
2018-2023

BER-SBR Vision Meeting Report 2018

New Approaches to Complex Environmental Systems

New Approaches to Complex Environmental and Collaboration Systems

Presentation Addresses Three Questions:

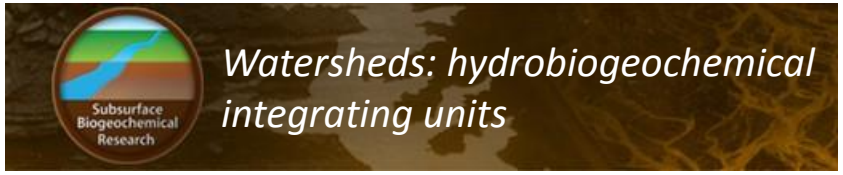
1. What are the scientific **objectives of the SBR program** and its component projects?
2. How are these scientific objectives being advanced through **three supporting elements**?
3. Can we enable innovation through community coordination – "**what could we advance together that would be difficult or impossible to do alone**"?
    - What are examples of current advances enabled through SBR-SFA based community efforts?
    - What are new opportunities to advance CESD innovation, including enhanced coordination and a few 'big ideas'.

Scientific Understanding to Enable Water and Energy Security

DOE Subsurface Biogeochemistry Program

Mechanistic understanding of flow and transport from molecular to watershed scales

- Addressing National Needs in:
  - Clean water availability
  - Contaminant management
  - Nutrient availability
  - Water-Energy



Three Key Elements enable coordination and innovation across SBR.....

Element 1: Crosscutting Scientific Questions

1. Quantify how biological behavior, abiotic-biotic interactions and **molecular transformations** control the mobility of contaminants, nutrients and critical biogeochemical elements

2. Quantify and predict how **hydrology drives fine-scale biogeochemical processes** in surface-subsurface systems

3. **Translate biogeochemical behavior across relevant molecular to watershed scales** to accurately and tractably predict flows of water, nutrients and contaminants

4. Identify, quantity, and predict **watershed responses to natural and anthropogenic perturbations** and shifts to new states

5. Translate predictive understanding of watershed system function and evolution into near and long term **energy and environmental strategies.**

CESD Strategic Plan Grand Challenges:

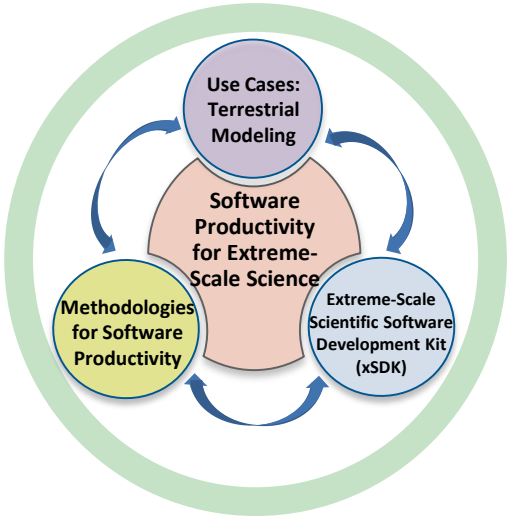
- **Biogeochemistry**
- **Integrated Water Cycle**

BERAC Grand Challenges:

- **Earth and Environmental Systems Sciences -** Hierarchy of models from process-resolving to reduced-order
- **Microbial to Earth System Pathways** – Define the key elements of microbial communities relevant for predicting larger-scale ecosystem phenomena

elements from ecosystems.

Element 2: Community Infrastructure for Data and Computation

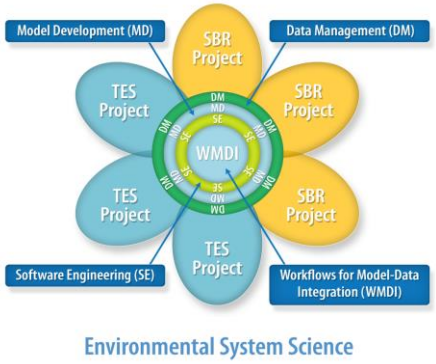


HPC computational infrastructure

Opportunity:

- Publish massive data sets **with interactive capabilities for analysis and visualization**
- Framework to enable easy **iteration between machine learning and mechanistic models**

Data Cyberinfrastructure



Environmental System Science

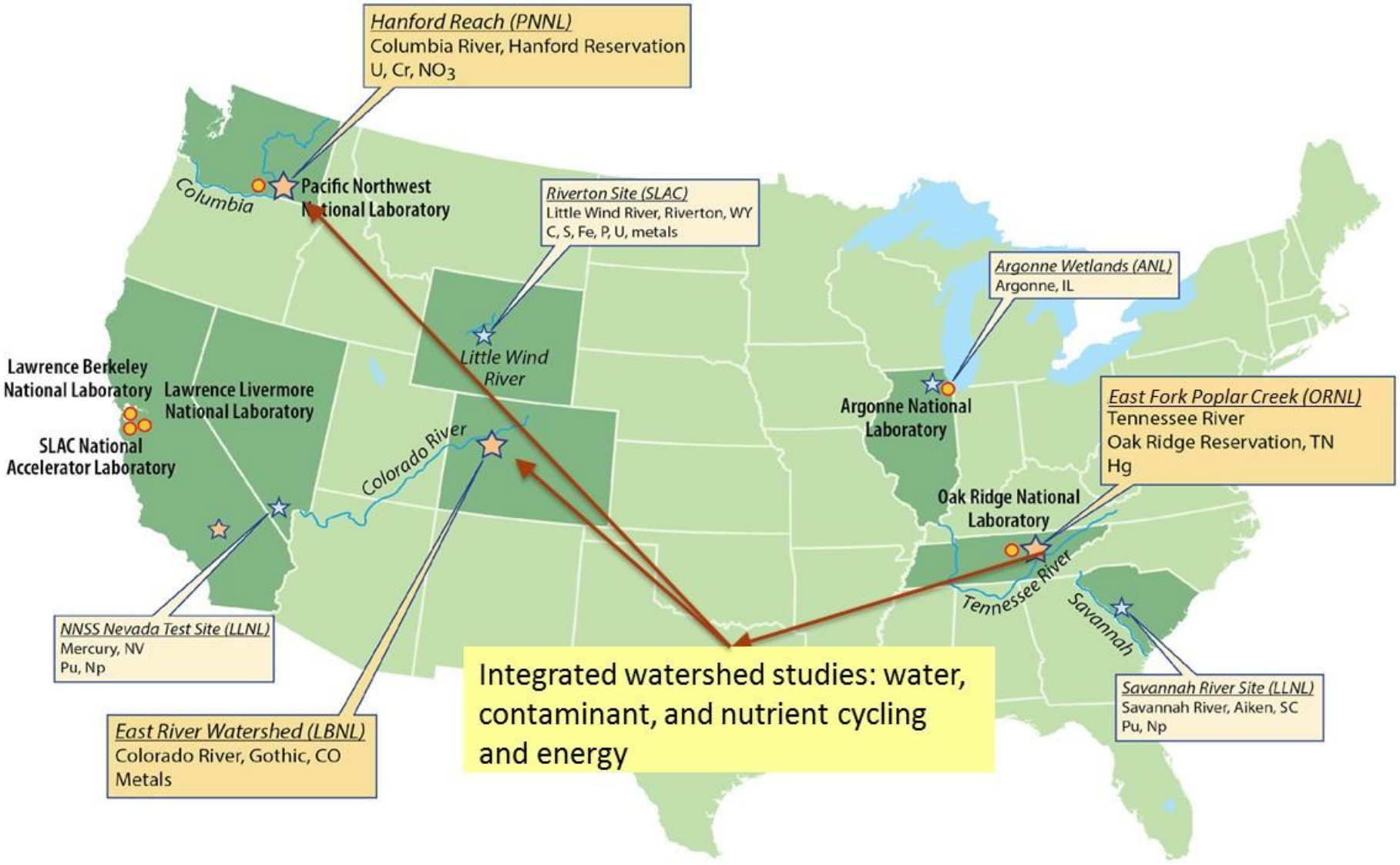
- Model intercomparisons /
- Input to ESS-Dive design
- Topical webinars and work
- Geospatial science to infor
- Exploring model-data integ

Opportunity:

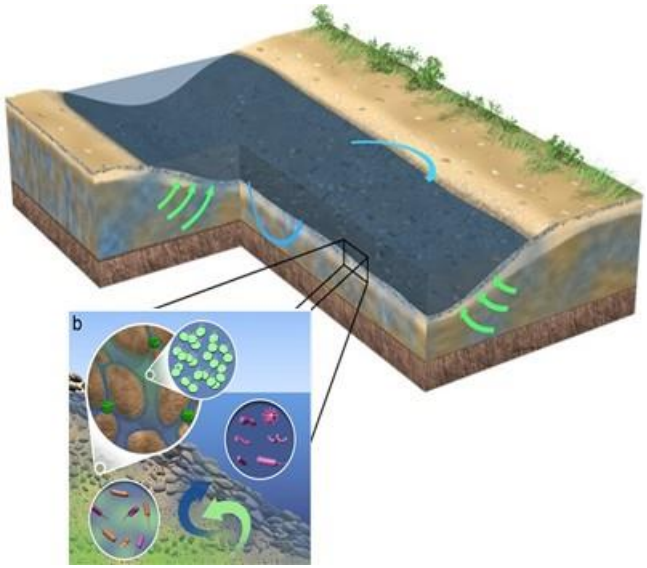
- Seamless data flow between ESS-Dive and K-Base to enable investigations of how biology shapes the environment and how the environment shapes biology

ESS Cyberinfrastructure Community Working Groups

Element 3: DOE-SBR Network of Complementary Testbeds



PNNL SBR SFA: Hydrobiogeochemistry of Managed Rivers and Watersheds



Understand the impacts of **river-groundwater exchange** flows on biogeochemical and ecological processes in the **Columbia River corridor**, and the resulting cumulative effects at the watershed scale

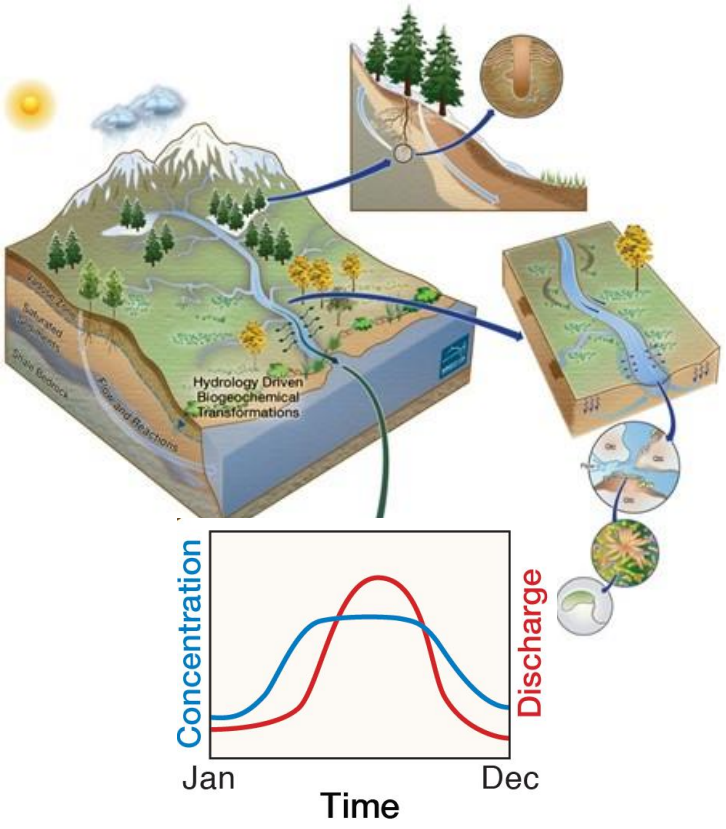
WHONDRS

Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems

WHONDRS seeks to broaden understanding of the impacts of river stage variability on exchange flows, biogeochemistry and ecology – beyond Columbia River research site.

Berkeley Lab Watershed Function SFA, East River CO

Testing Scale-Adaptive & System-of-Systems Approaches to Balance Complexity and Tractability, Upper Colorado River Basin



Predictive Understanding of how **Mountainous Watersheds respond to Perturbations** and **Retain and Release Water, Nutrients, Carbon and Metals** at **episodic to decadal** timescales

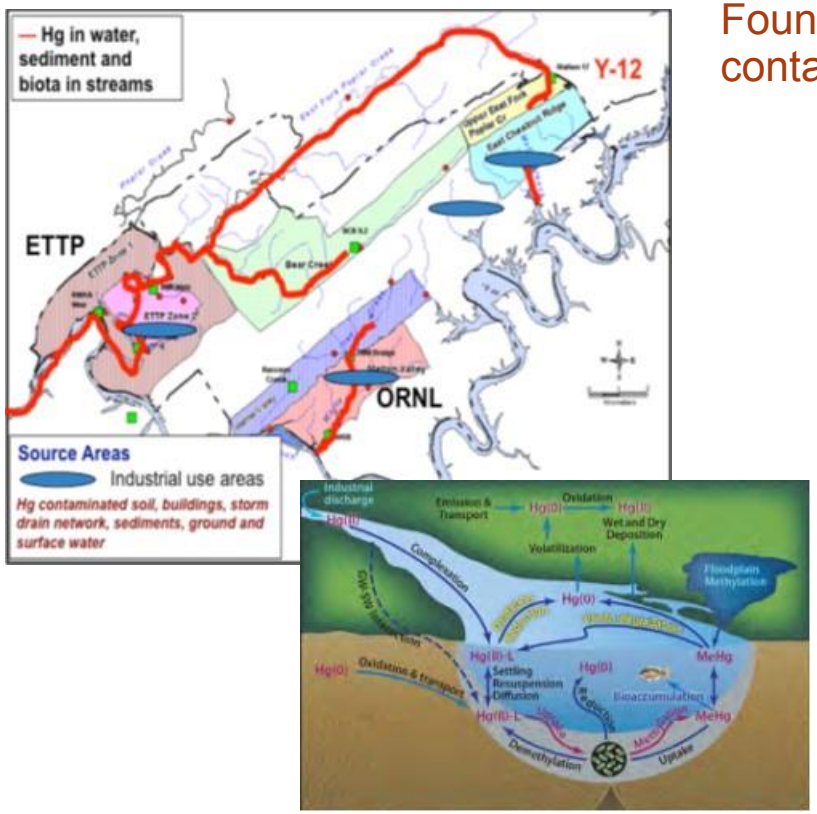
Community Bi-Monthly '**Community Watershed' Telecon** – Started in 2007; Over 225 current invitees.

Project has **hosted 450 individuals in CO Observatories** including researchers from:

- 7 countries and 33 US states
- 55 academic institutions,
- 16 federal, state and local government institutions (including USGS, NOAA, NASA, EPA)
- 13 private sector organizations.

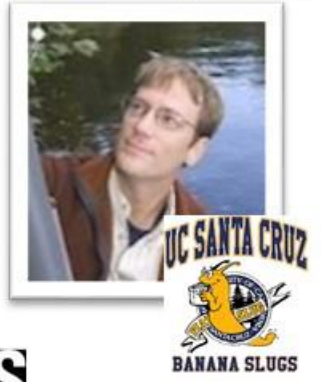
Collaboration Map based on recent Watershed Function SFA Publications

ORNL SFA: Biogeochemical Transformations at Critical Interfaces



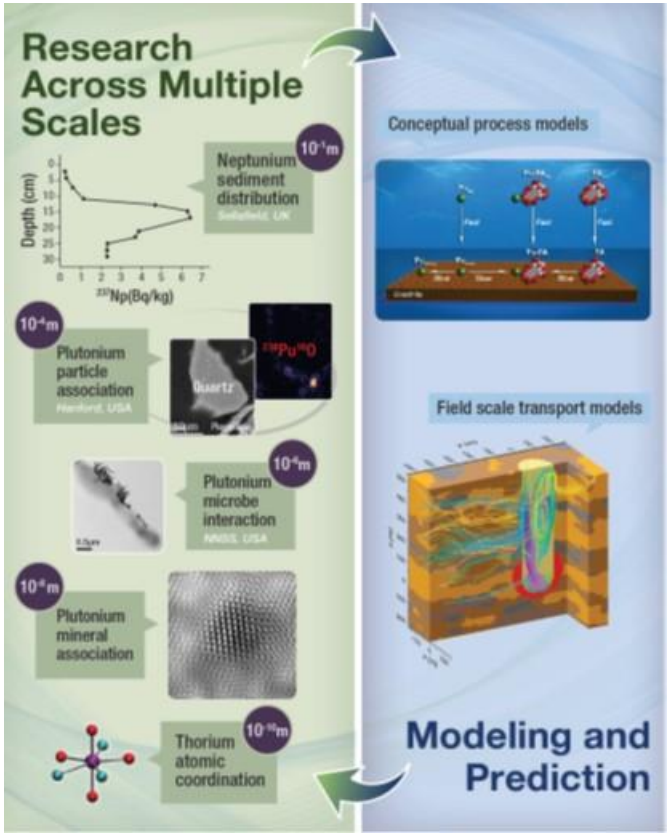
Foundational data to address Hg contamination globally (UNEP)

Applied new molecular probes for *hgcAB* genes to samples collected from a range of environments.



Determining the coupled hydrobiogeochemical processes controlling **mercury fate and transformation** in low-order freshwater stream systems

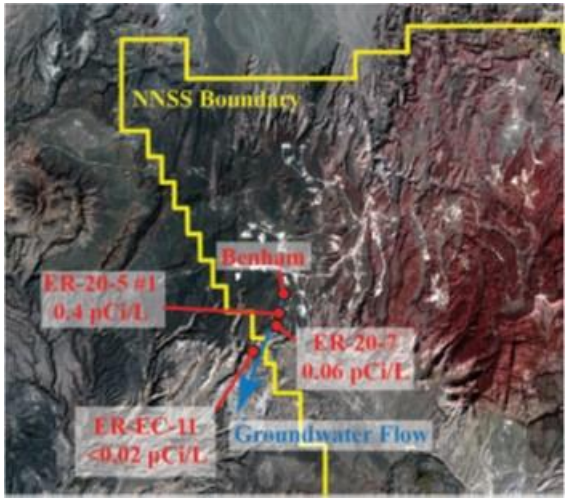
LLNL SFA: Subsurface Biogeochemistry of Actinides

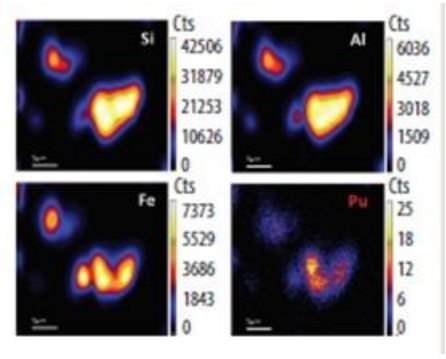


Building an understanding of actinide behavior from the atomic to field scale to improve prediction of actinide migration at globally relevant sites.

Community science at expanded testbed sites:

- NNSS
- SRS
- Hanford
- Sellafield/Ravenglass estuary -



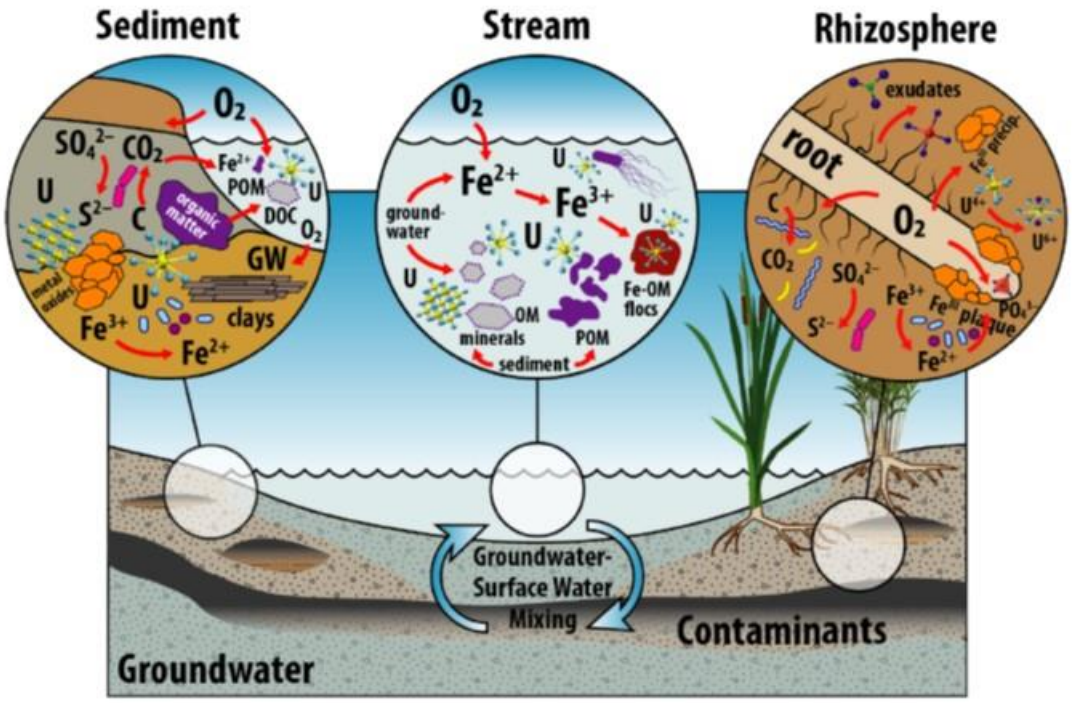


Nano-SIMS

State-of-the-art capabilities to detect and measure actinides

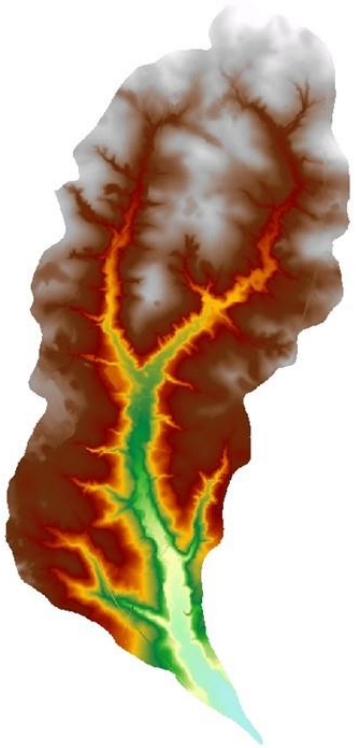
- Open to the SBR community
- Can accept radioactive samples
- Used by research groups worldwide

ANL SFA: Wetland Hydrobiogeochemistry



Development of a mechanistic understanding and ability to model the coupled hydrological, geochemical, and biological processes controlling water quality in wetlands and the implications of these processes for watersheds commonly found in humid regions of the United States.

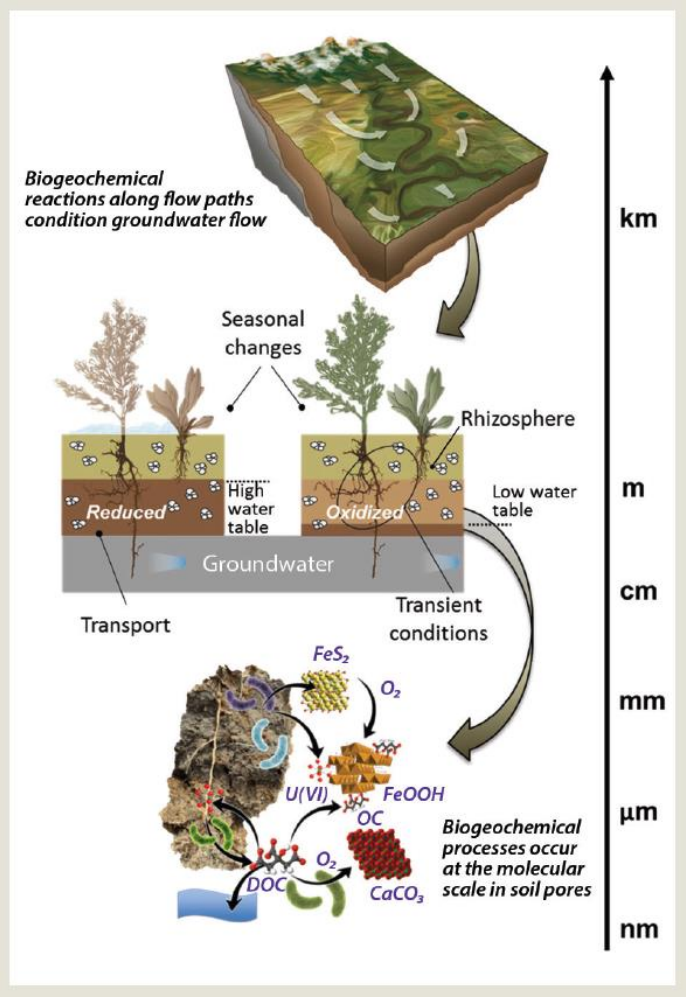
New testbed site at Savannah River Site: Tims Branch Watershed



Collaborative network of participants:

- Clemson
- FIU
- PNNL (EMSL)
- Korea Univ.
- China Univ. of Geosci.
- Universidade Federal de Alfenas
- LBNL (Enigma, Kbase)
- Univ. of Leeds

SLAC SFA: Groundwater Quality



Advancing predictive understanding of hydrologically driven biogeochemical processes in the capillary fringe controlling water quality

Community advancement of synchrotron-based approaches for application to biological and environmental research.

- **Synchrotron Environmental Science (SES) Conference** series held at synchrotrons to further integration between synchrotron and environmental scientists.
- **Envirosync**- voice to federal agencies for Biological and Environmental Scientists who use synchrotron radiation in their research.

Opportunities and Big Ideas for Discussion and Feedback

Strategic Synchrotron Community Advances for Biogeochemistry

Unparalleled biogeochemical characterization across Synchrotrons:

- Infrared nano-spectroscopic imaging (ALS)
- Hard X-ray *nano*probe (NSLS-II)
- Fluorescence-based 3D X-ray microscopy (APS)
- Infrared spectro-microtomography (ALS)
- Machine learning data mining of 2D and 3D image data (SSRL)
- Cryo-electron tomography for protein imaging (SLAC)

Meet with BER synchrotron reps Wednesday, 12pm-1pm

- **ALS-; psnico@lbl.gov, hyholman@lbl.gov**
- **APS-; kemner@anl.gov**
- **NSLS-II -; rtappero@bnl.gov**
- **SSRL-; bargar@slac.stanford.edu**

Opportunity: Collection and Analysis of **Common Suite** of Environmental Biogeochemical Measurements,

Acquisition and analysis coordinated across **SBR Observatories** and **Synchrotrons**

….and **EMSL, JGI**

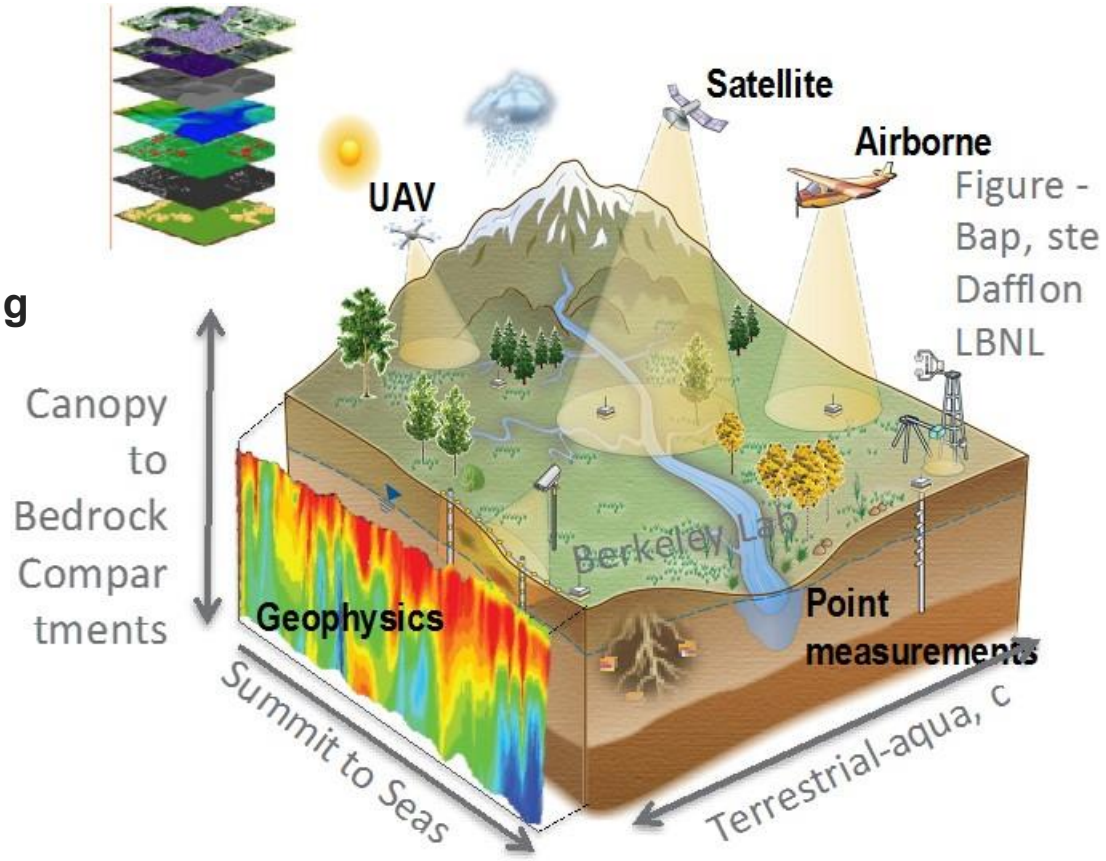
Opportunity: Linkages with User Facilities and User Programs

Opportunity:
Iterative Model-Experiment Integration Across Scales (MODEX)

Meet representatives on Wednesday, 12pm-1pm

Opportunity: 4D Watershed Imaging

- Monitoring of **vegetation, microbial ecology, biogeochemistry, hydrogeology & geochemistry** watershed dynamics through **integrating direct and proxy measurements**
- **Networking** of increasingly **autonomous sens**ors
- **Novel sensors** (biosensors, root imaging, optodes & quantum-based, etc.).
- **Machine learning** to rapidly explore diverse datasets and identify hot spots and moments



Opportunity:
Coordinated ESS effort to develop unparalleled capacity to "watch" watersheds function in real time and to rapidly assimilate information into predictive models

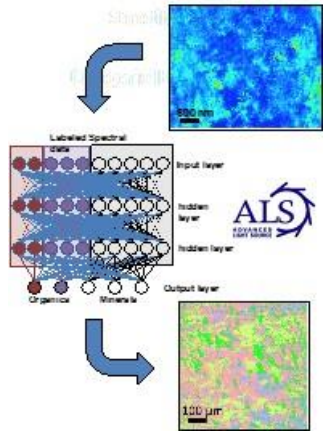
Opportunity: Machine Learning for the Environment

- Many recent advances by SBR investigators

Opportunities:

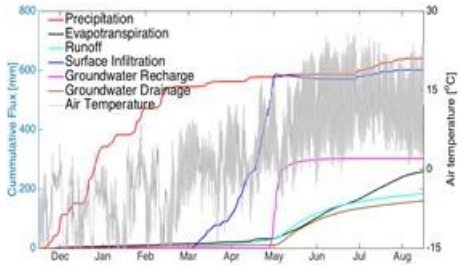
- Significant potential for improved:
  - Cross-scale, cross-compartment imaging
  - Conceptual model development
  - Model-data integration
  - Assimilation of field streaming data into models

- IDEAS-like framework for data-driven environmental tools and model-data integration frameworks



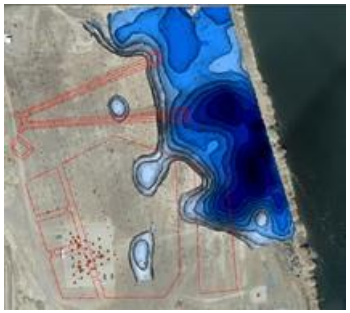
Linking synchrotron information about shale chemical heterogeneity across nano- and micro-scales

Hao et al., Nature Scientific Reports, 2018



Estimating water partitioning through assimilation of daily autonomous ERT field data into coupled model

Tran et al., in review

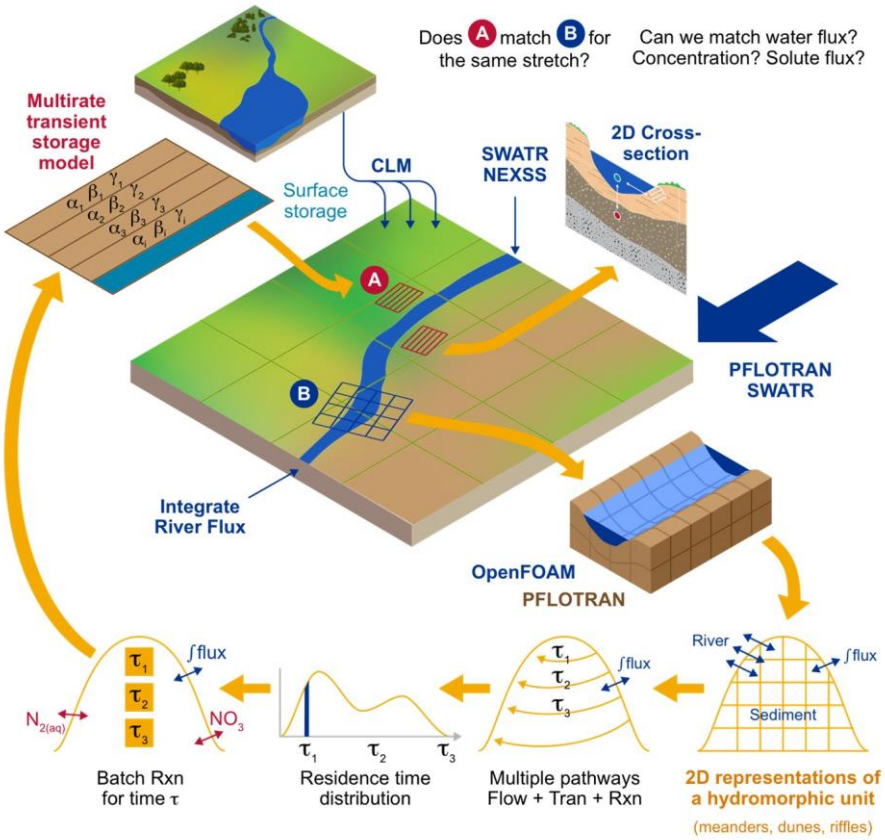


Linking groundwater time-series data with patterns of river water intrusion using deep learning

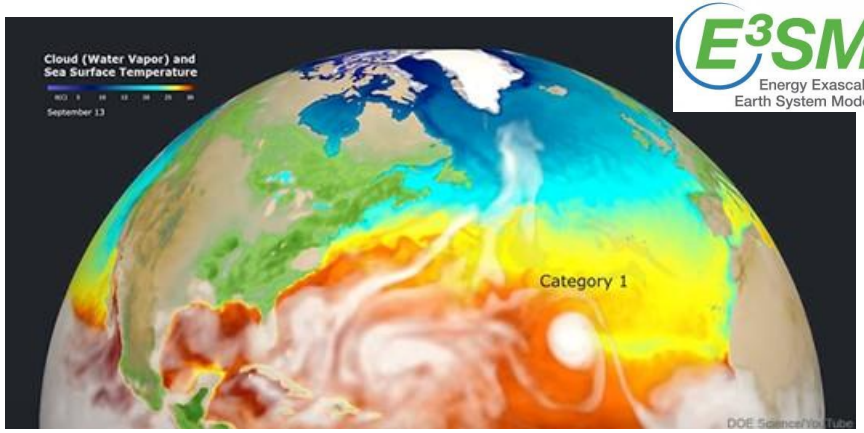
X. Chen with PNNL Deep Science Initiative

Opportunity: Cross-BER Program Linkages

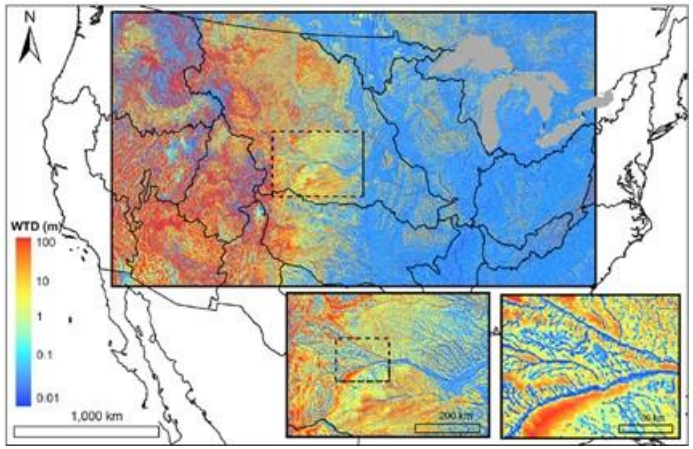
Opportunity: Integration of top-down and mechanistic approaches to Earth Systems modeling across ESS and E3SM



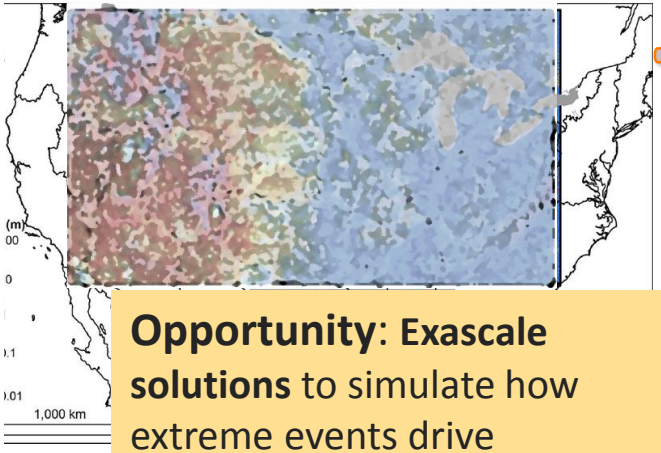
Big Idea: Quantifying Influence of Extreme Events on Watershed Hydro-Biogeochemistry across CONUS



E3SM for predicting future climate and weather variability



Maxwell et al., 2015 Prediction of surface-groundwater interactions across the CONUS



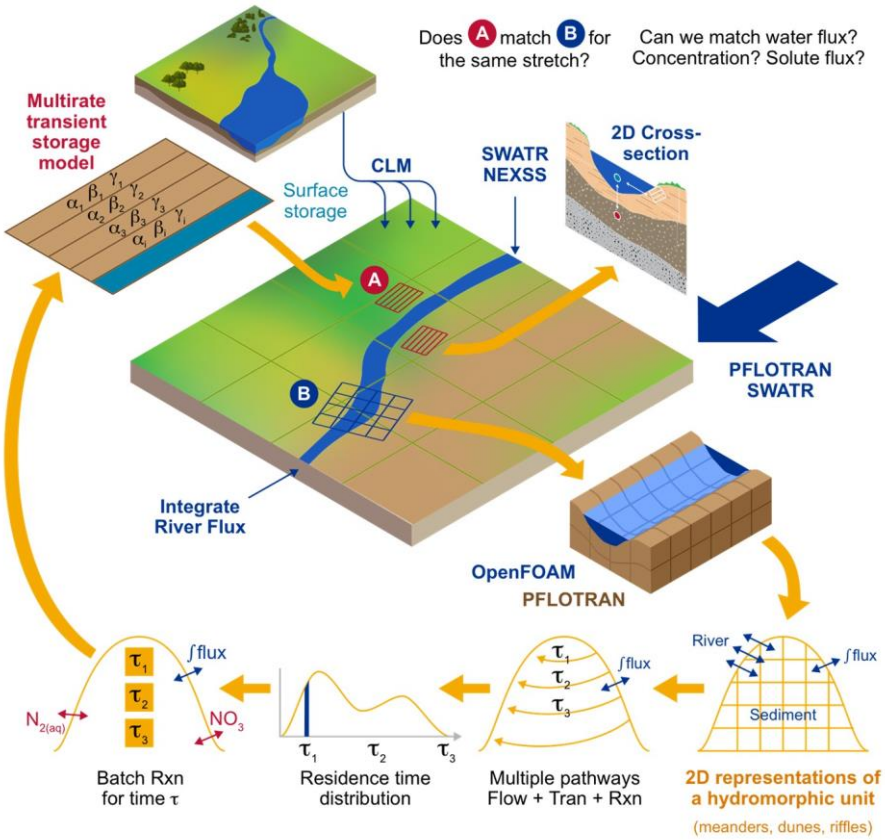
Opportunity: **Exascale solutions** to simulate how extreme events drive **biogeochemical cycles across CONUS**

Opportunity: **SBR observatories coordinate** assessment of how **extreme events manifest** in different key US watersheds

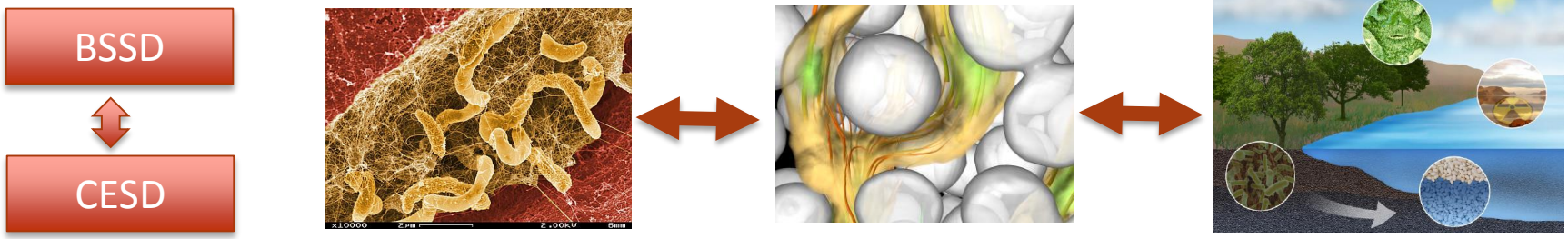
Predictive understanding of impacts of bomb cyclones, western droughts, Atm rivers and other extreme events on **US energy, water availability, nutrients and contaminant mobility**

Opportunity: Cross-BER Program Linkages

Opportunity: Integration of top-down and mechanistic approaches to Earth Systems modeling across ESS and E3SM

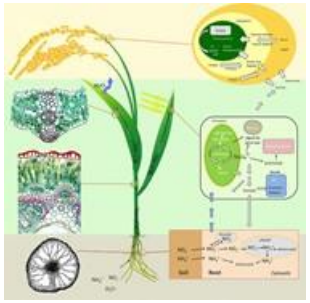


Opportunity: Integrating **microbial and plant biological understanding** into earth and environmental systems models

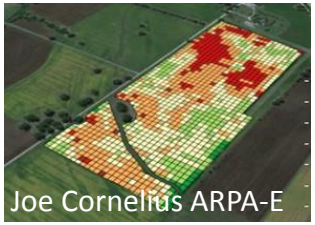


Big Idea - Managed Biosystems: Realizing the potential of G x E x M with designer crops in novel environments to meet future Energy and Food Demands

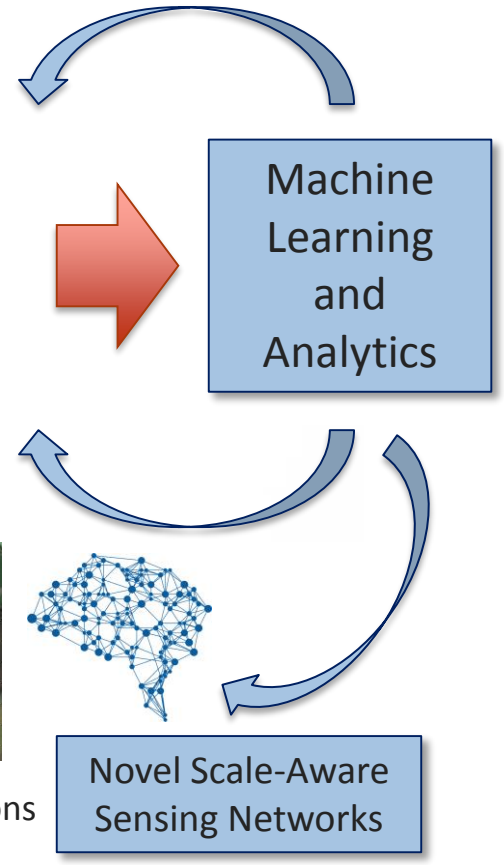
Genome-Based Trait Associations



Virtual Plant Model



Environmental Variations and Perturbations



G (Genotype) x E (Environment) x M (Management)
Mechanistic Models to Predict System Performance

Opportunity:

- Multiscale approach to biodesign and management
- Virtual plant model for many combinations of G x E
- Machine learning / big data analytics to identify interesting combinations of genotype and environment
- Iterate with modeling/experiments
- Define optimal management strategies

Opportunity: Network of Networks

NSF and International ESS Networks

neon
National Ecological Observatory Network

LTER NETWORK

TERENO
TERRESTRIAL ENVIRONMENTAL OBSERVATORIES

OZCAR

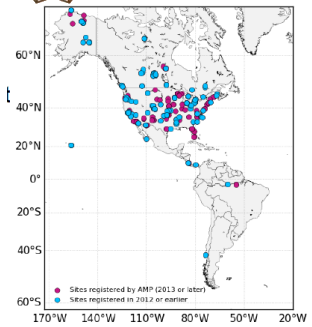
Opportunities:

- US Integrated Field Laboratories (IFLs)– measurements across gradients and compartments
- Global network to address gaps and challenge models

DOE Networks

Subsurface Biogeochemical Research

AMERIFLUX MANAGEMENT PROJECT



"Yes, and…"

Thanks to SBR Leads for their Input:


Annie Kersting
LLNL


Eric Pierce
ORNL


John Bargar
SLAC

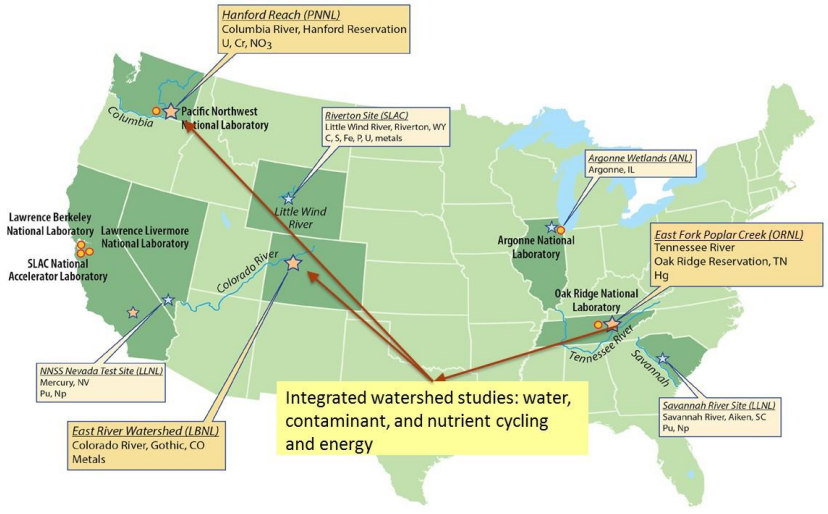

Ken Kemner
ANL

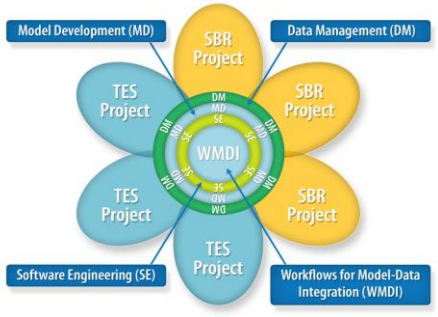
JGI JOINT GENOME INSTITUTE DEPARTMENT OF ENERGY

ARM CLIMATE RESEARCH FACILITY

KBase

EMSL





Environmental System Science