Subsurface Biogeochemical Research

SBR/TES Joint Investigators Meeting

May 19, 2020

Paul Bayer, EESSD

Jennifer Arrigo, EESSD

Amy Swain, BSSD

Welcome

Jennifer Arrigo

Joins ESS team from the U.S. Global Change Research Program's (USGCRP) National Coordination Office

Co-managing SBR + Other

Formerly

- Manager, Climate Monitoring Program (NOAA)
- Deputy Director, Consortium of Universities for the Advancement of Hydrologic Sciences, Inc. (CUAHSI)
- Assistant Professor, Atmospheric Sciences (East Carolina University)

- Welcome

2020 ESS PI Meeting Abstract Book

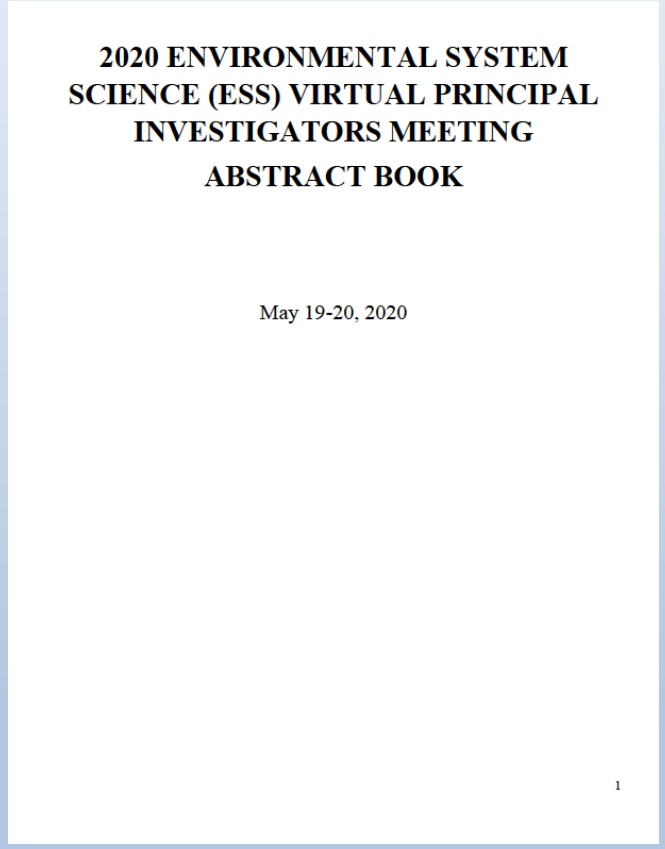
Uploaded to the original ORISE Registration Page

https://www.orau.gov/2020esspi/abstract-book.htm

Also uploaded to the SBR and TES web pages

SBR - https://doesbr.org/PImeetings/index.shtml

TES - https://tes.science.energy.gov/PImeetings/index.shtml



2020 ENVIRONMENTAL SYSTEM SCIENCE (ESS) VIRTUAL PRINCIPAL INVESTIGATORS MEETING

ABSTRACT BOOK

May 19-20, 2020

1

PI Awards and Publications

2019-2020

European Association of Geochemistry, H.C. Urey Award
J. Banfield (UC Berkeley) – 2020

Fellows
T. Bianchi (U. Florida) – 2019
R. Maxwell (CSM) – 2019
C. Steefel (LBNL) - 2019

2020 Darcy Lecturer
Reed Maxwell (CSM) - 2020

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES
International Fellow
K. Maher (LBNL) – 2020

Academy Member
S. Hubbard (LBNL) – 2019

AAAS Fellow
A. Wolfe (ORNL) – 2019

Geochemical Society – Fellows
B. Gu (ORNL) - 2020

Geochemical Society – Exec Editor GCA
J. Catalano (Washington U.)

Fellows
D. Gochis (UCAR) – 2019

Member
S. Hubbard (LBNL) – 2020

Fellowship, Univ Salzburg
I. Larsen (U. Mass) – 2020

30 Under 30 List
F. Maina (LBNL) – 2020

Engineering Alumni Assoc
L. Li (Penn State) – 2019

Robert G. Wetzel Award
S. Hubbard (LBNL) – 2019

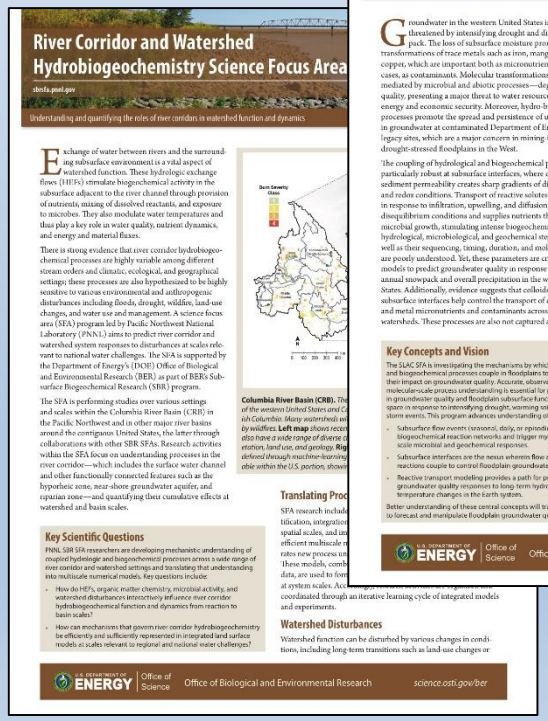
- 123 publications in 2018
- 103 publications in 2019
- 32 publications (so far) in 2020

American Academy of Microbiology Fellow
M. Podar (ORNL) – 2020

Updated SBR SFA Flyers

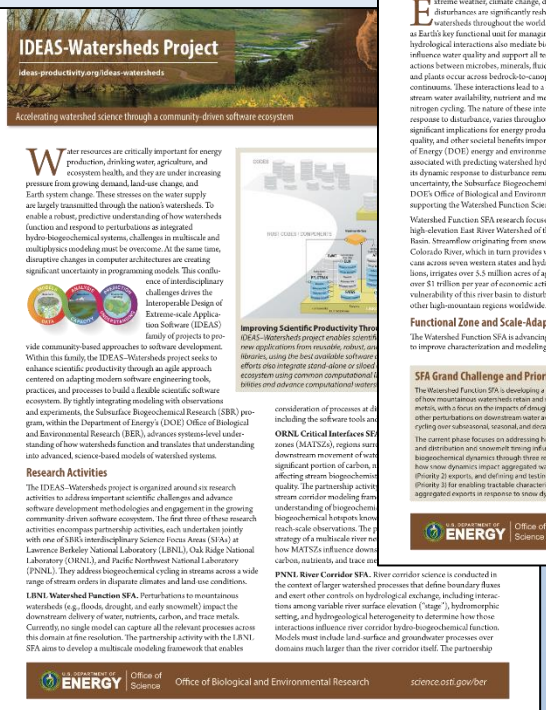
2020

PNNL SFA



SLAC SFA

IDEAS-W Project



LBNL SFA

https://doesbr.org/research/sfa/index.shtml

Earth and Environmental Systems Sciences Division Strategic Plan

Vision: Develop an improved capability for Earth system prediction on seasonal to multi-decadal time scales to inform the development of resilient U.S. energy strategies.

High level Grand Challenges

- **Integrated water cycle** – processes involving atmospheric, terrestrial, oceanic and human system components and their interactions and feedbacks across local, regional and global scales.
- **Biogeochemistry** – coupled biogeochemical processes and cycles across spatial and temporal scales by investigating natural and anthropogenic interactions and feedbacks.
- High Latitudes – quantify the drivers, interactions and feedbacks among the high latitude components and between the high latitudes and the global system.
- Drivers/Responses in the Earth System – next generation understanding of Earth system drivers and their effects on the integrated Earth-energy-human system.
- **Data-Model Integration –** develop a broad range of interconnected infrastructure capabilities and tools that support integration and management of models, experiments, and observations across a hierarchy of scales and complexity.

SBR Program Goals and Objectives

Goal: The SBR program seeks to advance a robust predictive understanding of how watersheds function as integrated hydro-biogeochemical systems and how these systems respond to perturbations such as changes in water recharge, availability and quality; contaminant transformation and transport; nutrient loading and cycling; land use and vegetative cover.

Five Priority Research Objectives:

- Quantify and predict the mechanisms by which hydrology drives fine scale biogeochemical processes and the exchange of water in coupled surface-subsurface systems;
- Quantify how biological behavior and feedbacks and abiotic-biotic interactions leading to molecular transformations influence mobility, transformation, fluxes, cycling, and fate of key nutrients (e.g., N, P, C), inorganic elements (e.g., S, Fe, Mn), and legacy DOE contaminants (e.g., U, Tc, Hg);
- Translate biogeochemical behavior across relevant molecular to watershed scales to accurately and tractably predict flows of water, nutrients, and contaminants;
- Identify, quantify and predict watershed response to natural and anthropogenic perturbations and shifts to new states; and
- Translate predictive understanding of watershed system function and evolution into near- and long-term environmental and energy strategies.

Understanding Integrated Watershed Function

Hydro-biogeochemical Processes

How "watersheds function"

- Structure underpins function
- Function (static) and dynamics
  - Headwaters to the mouth

"Integrated Systems"

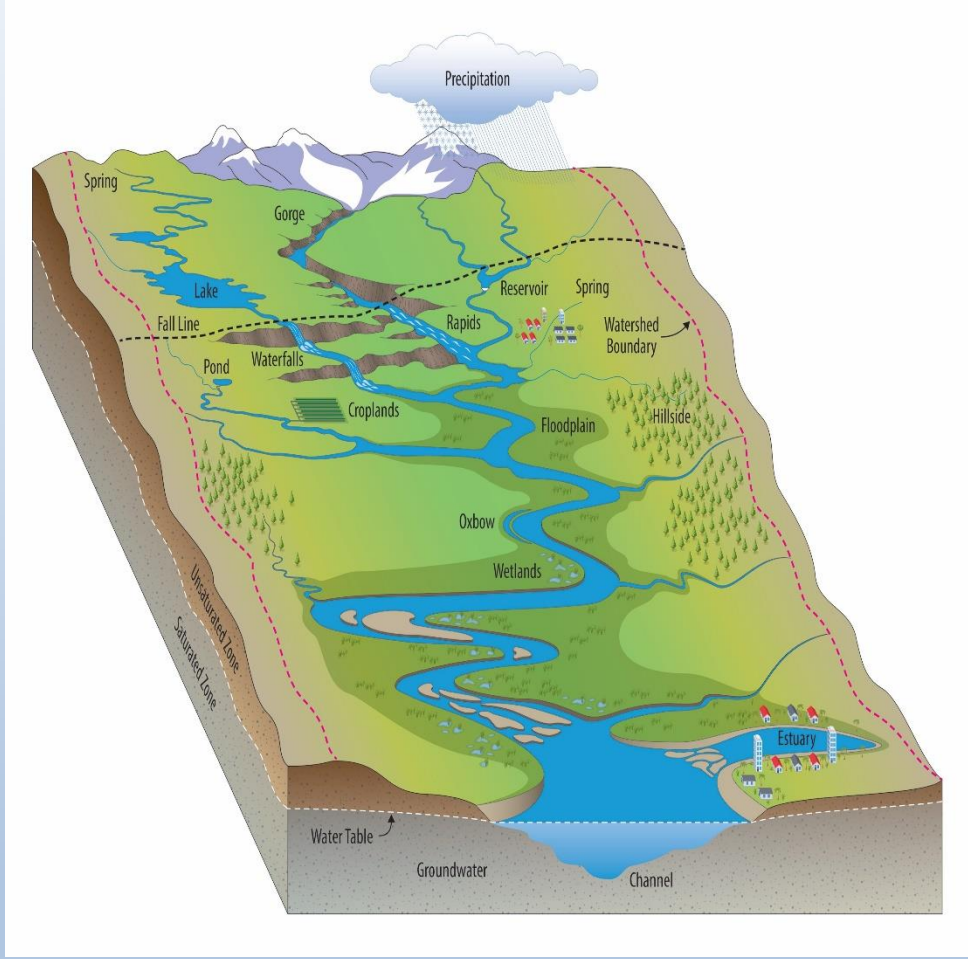
- Surface to subsurface processes

"Hydro-biogeochemical Systems"

- Scales of research
  - Molecular to watershed/basin
- Biotic to abiotic
- Key elements, nutrients, contaminants
  - BGC cycling and transport

"Response to perturbations"

- Water recharge, availability, quality
- Contaminant transformation and transport
- Nutrient loading and cycling
- Land use/change and vegetation cover



"Predictive Understanding"

- Interoperable codes to capture multi-temporal and spatial scales

SBR Science Focus Areas

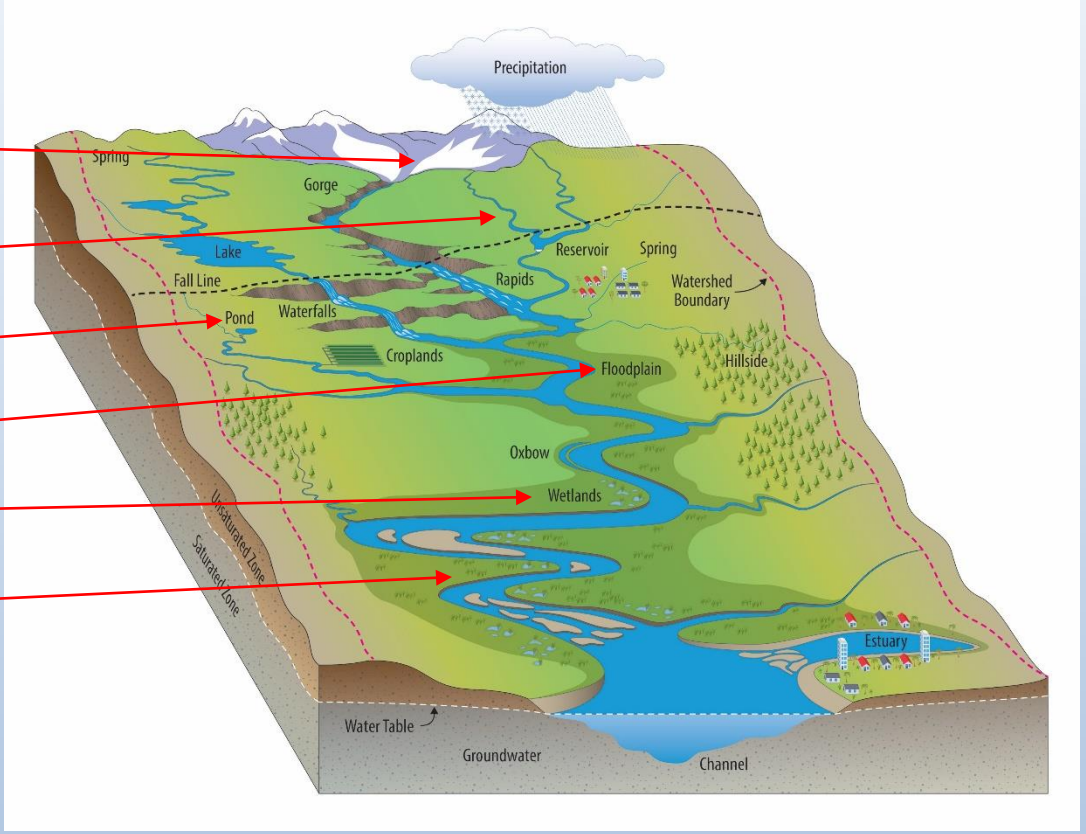
- **LBNL: Watershed Function ($6.8M)**
  - Hydro-biogeochemical dynamics from genome to watershed scales.
- **PNNL: River Corridor and Watershed Hydro-BGC ($5M)**
  - Understanding of coupled hydrologic and biogeochemical processes in large, dynamic rivers and associated watersheds and translating that understanding into multi-scale numerical models.
- **ORNL: Biogeochemical Transformations at Crit. Interfaces ($3.5M)**
  - Determining the coupled hydro-biogeochemical processes controlling mercury transformations in metabolically active transient storage zones in low-order freshwater stream systems.
- **ANL: Wetland Hydro-Biogeochemistry ($1.2M)**
  - Understanding the mechanisms of hydrologically-driven molecular- to core-scale biogeochemical transformations within redox-dynamic environments and the effect of hydrologically-driven Fe and S biogeochemistry on water quality.
- **LLNL: BioGeoChemistry of Actinides ($1.1M)**
  - Understanding surface and subsurface actinide behavior to provide a basis for managing transport phenomena and long-term stewardship.
- **SLAC: Groundwater Quality ($1M)**
  - Investigating the coupling of fine-scale hydrologic and biogeochemical processes in transiently saturated zones and impacts on water quality.

Understanding Integrated Watershed Function

Hydro-biogeochemical Processes

Existing Watershed Testbeds (Res Area 3):

- Mountainous headwaters (LBNL)
- 3rd order stream (ORNL)
- Ponds/Lakes (LLNL)
- Alluvial floodplain (SLAC)
- Wetlands (ANL/SRNL)
- 8th order river (PNNL)



Novel Structural Components of Watersheds (Res Area 4):

- Springs
- Gaining/Losing parts of streams
- Mouth of watersheds

FY19/FY20 SBR-Relevant Solicitations

FY19 ESS FOA 2035

- Two Topics:
  - Ecohydrology/Hydro-biogeochemistry
  - Geochemistry/Biogeochemistry
- Limitations:
  - Complementary to the SBR SFAs
  - Within the contiguous U.S.
- Awards
  - S. Fendorf (Stanford U.), DOM in floodplains (ANL, LBNL, PNNL)
  - M. Ginder-Vogel (U. Wisconsin), Particulate OM (PNNL)
  - Mike Goosef (U. Colorado), Groundwater inflows (PNNL)
  - C. Santelli (U. Minnesota), Fe-S-C cycling in wetlands (ANL)
  - L. Li (Penn State U.), Watershed-scale rate law for chemical weathering and nutrient export (LBNL)

FY20 ESS FOA 2184

- Two TES and Two SBR Topics:
  - Sci Area 3 – Existing Watershed Testbeds
  - Sci Area 4 – Novel Structural Components of Watersheds (Springs, Gaining/Losing stretches and Mouth)
- Limitations:
  - Sci Area 3 – Complementary to SFAs & Exploratory only
  - Both - within the continental U.S.
- SBR Review Panels May 5 and May 7-8, 2020
- Evaluating reviewer comments

FY19 ESS Early Career Solicitation

BER Early Career Solicitation FOA 2019 and Lab 19-2019

- BSSD & EESSD Topics – ESS for FY19
  - Limitations:
    - Complementary to the SBR and TES SFAs or major research projects
    - Within the U.S.
  - Awards:
    - Isaac Larsen, U. Massachusetts, Amherst
      - Abiotic and Biotic Controls on Chemical Weathering Rates and Solute Generation
    - James Stegen, PNNL
      - Multi-Watershed Perturbation-Response Traits Derived Through Ecological Theory
    - Charuleka Varadharajan, LBNL
      - Investigating the Impacts of Streamflow Disturbances on Water Quality using a Data-driven Framework
  - Congratulations!

EPSCoR - Established Program to Stimulate Competitive Research

https://science.osti.gov/bes/epscor

FY20 FOA2215 - applications submitted April 7, 2020 (extended)

Federal-State Partnership Program

- Designed to enhance the capabilities of designated states and territories to conduct sustainable and nationally competitive energy-related research
- 25 eligible states plus Puerto Rico, Guam and the U.S. Virgin Islands
- Support fundamental, early-stage energy research collaborations with the DOE national laboratories
- Any research areas relevant to an SC program. Special emphasis on:
  - QIS, Microelectronics, Data science/ML/AI, Energy storage, Plastics recycling

Project Funding

- $150K - $250K/year
- Aligned program kicks in 10% of the cost/year

Program Manager (BES) – Tim Fitzsimmons

ESS POC – Paul Bayer

Selections

- FY20 ESS-relevant applications - 6, one split with MSD
- FY19 ESS-relevant applications - 3, none selected
- FY18 ESS-relevant applications – 5, one selected (Rishi Parashar, DRI)

Award Search

https://pamspublic.science.energy.gov/WebPAMSExternal/interface/awards/AwardSearchExternal.aspx

FOA Requirements and Limitations may vary from year to year

FY20 SBR-Oriented SBIR/STTR Solicitation

- **Small Business Innovation Research (SBIR)/Small Business Technology Transfer (STTR)**
  - Annual Solicitation for Phase I, $200K/1 yr projects
    - FY20 FOA2145 issued August 12, 2019.
    - Topic 26 - Technologies for Characterizing and Monitoring the Subsurface, Terrestrial Ecosystems and Watersheds
    - Two subtopics
      - Real-Time, In-situ Measurements of Hydro-biogeochemical and Microbial Processes in Watersheds and Subsurface Systems – 11 awards
      - Image Processing Improvements for In Situ Fine Root Measurements – 5 awards
  - Annual Solicitation for Phase IIA and IIB, $1.1M/2 yr projects
    - FY20 FOA2155 issued October 22, 2019
    - IIA – within original scope; IIB – extension of original scope
    - ESS awards:
      - Vista Clara (E. Grunewald) - Switched-Field Surface NMR for Groundwater Resolution
      - Innovative Wireless (M. Fisher) - Integrated Env. Quality Sensing System (IEQS)
      - Physical Sciences (D. Sonnenfroh) - Ultra-compact Laser Ceilometer for Boundary Layer and Cloud Height Retrievals
    - CARES Act
      - InnoSense (A. Ray) - Portable Nanowire Platform for Quasi Real-Time and Ultrasensitive Detection of Microbes

SC Graduate Student Research (SCGSR) Program

http://science.osti.gov/wdts/scgsr/

2020 Solicitation 1: Due May 20, 2020 (extended)

Supplemental Awards

3-12 months conducting part of a doctoral thesis/dissertation research at a DOE lab (not the same as a field site)

Collaborate with a DOE laboratory scientist

BER Coordinator – Jay Hnilo

Environmental System Science - SBR

FY19, Round 1 (SBR)

-No awards

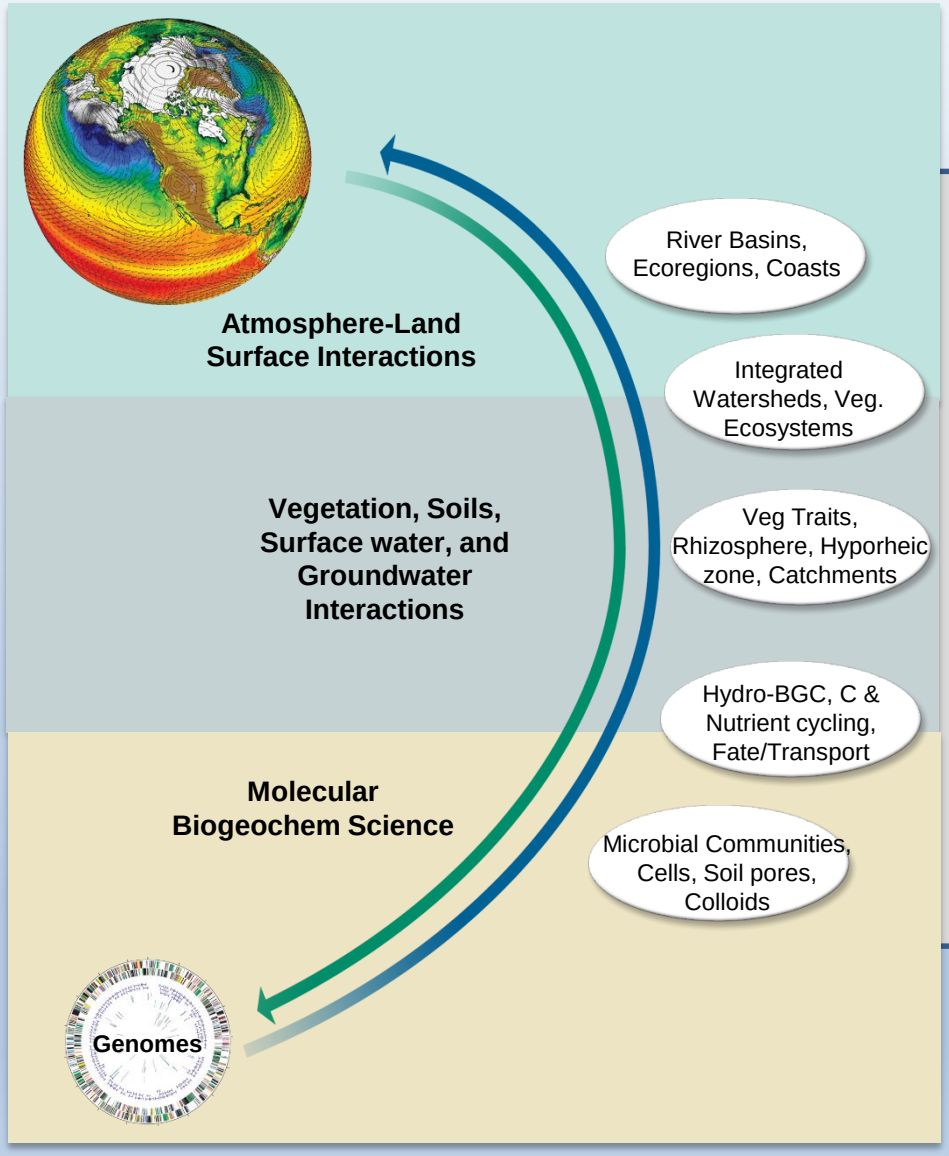
FY19, Round 2 (SBR)

- C. Anderson, U. Massachusetts-Amherst (E. Brodie, LBNL) - Deciphering metabolic constraints on soil carbon oxidation in hydrodynamic floodplain soils using an integrated multi-omics approach
- J. Stoll, Kent State University (S. Brooks, ORNL) – Direct and Indirect Effects of Micronutrients on Methyl Mercury Production

FY20, Round 1

-Due May 20, 2020

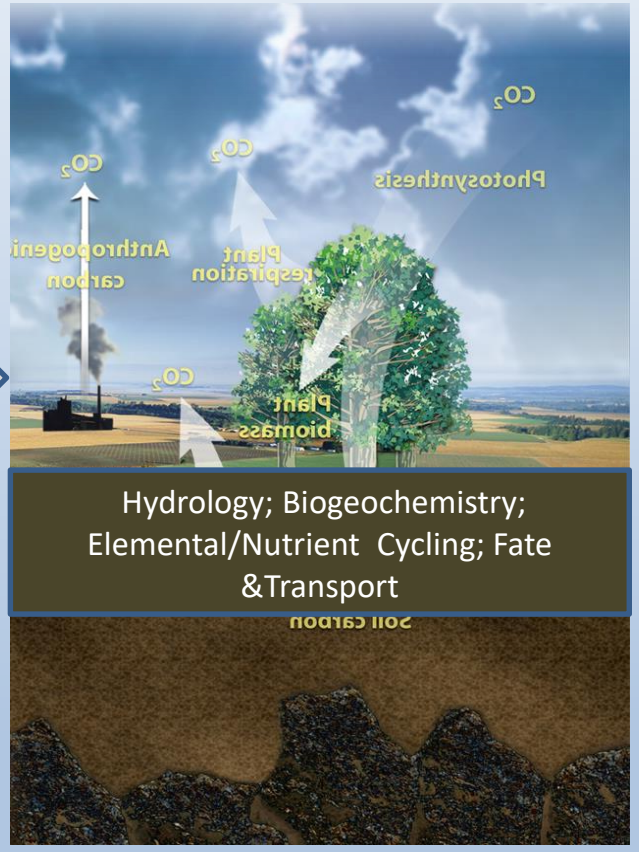
Scales of BER Systems Science & ESS Scope



ESS Scope

TES

(Canopy=>Soils, Roots)



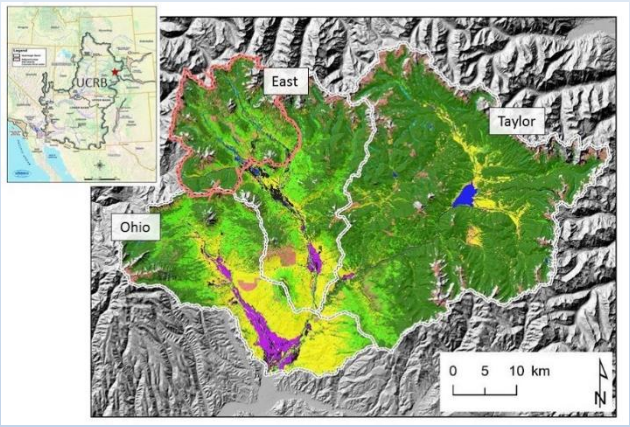
SBR

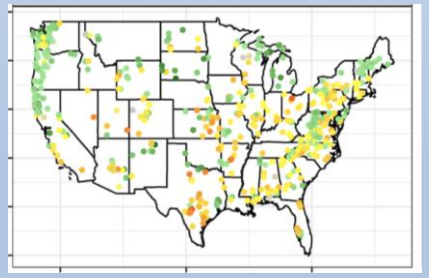
(Watersheds=>Soils, Sediments, Groundwater)

ExaSheds Pilot Project

ExaSheds Pilot: To advance Watershed System Science using Machine Learning and Data-Intensive Extreme-Scale Simulation

- Pilot initiated in 2019, 4 labs
- Co-led by C. Steefel (LBNL) and Scott Painter (ORNL)
- Funded by Data Management (J. Hnilo)
- Exploring strategies for learning-assisted simulation
  - Development of model inputs from sparse, coarse and indirectly-related information
  - Hybridization of process-resolving simulations and ML
- Working with data from:
  - East River, Colorado
  - Upper Colorado Water Resources Region
  - Continental U.S.
- Adapting DOE-developed watershed simulation tools to leadership-class computer architectures

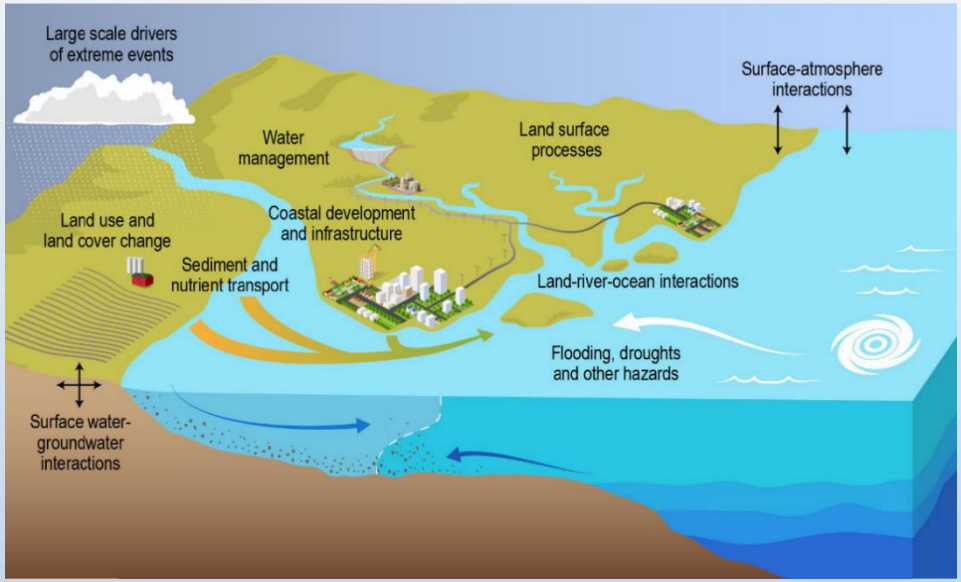




ExaSheds

Integrated Coastal Modeling (ICoM) Project

"Deliver a robust predictive understanding of coastal evolution that accounts for the complex, multiscale interactions among physical, biological, and human systems."

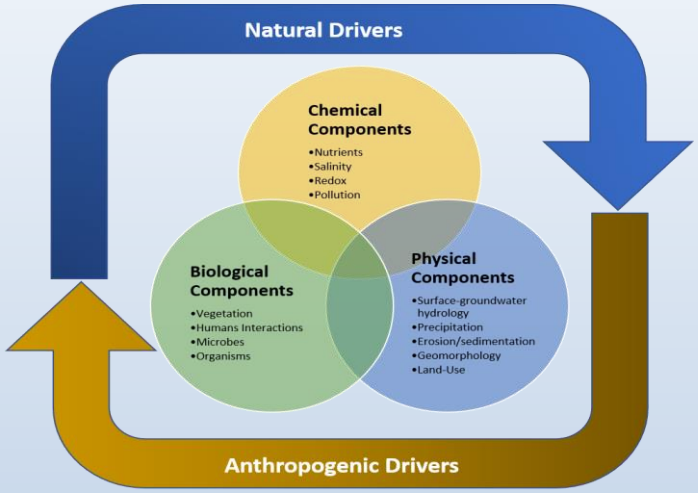


- **PNNL-led multi-institutional team** (LANL a major participant)…>40% funding awarded by PNNL to others
- **Mid-Atlantic regional focus** … existing DOE capabilities, complex systems interactions, extensive data, and converging interagency activities
- **$16.2M** over three years ($5.4M/yr)
- **SBR ($200K/yr)** to D. Moulton (LANL) for SW/GW interactions and coastal flooding.
- **A "federated" approach** spanning four distinct program areas within DOE's CESD; requires foundational work in each area and substantial crosscut modeling work.
- **Informs potential follow-on observational and experimental work.**

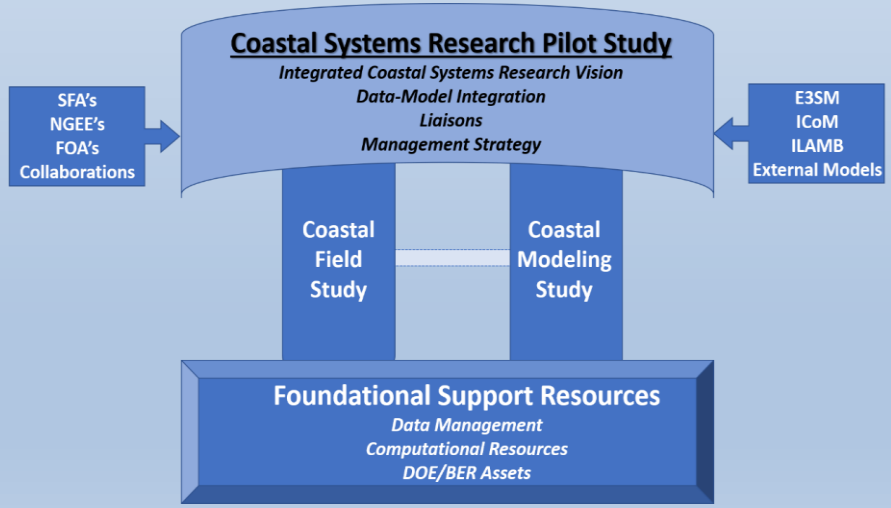
New EESSD "Coastal Systems" Project

FY20 Appropriation

- Congressional direction to fund PNNL
- Most of the EESSD program managers will be involved in preparing guidance and in the future peer review process:
  - Dan Stover – leads team (mostly ESS PMs) for the field research/process modeling study
  - Renu Joseph – leads team (mostly EES modeling PMs) for the Great lakes regional modeling effort.
- Includes funding for mid-range compute resources, data management and software liaisons.



Coastal system components and drivers

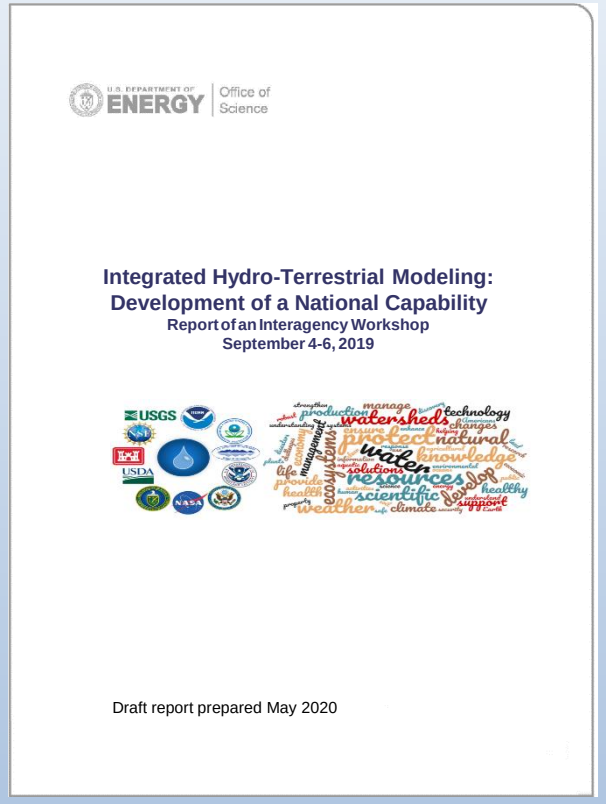


Conceptual diagram of project structure

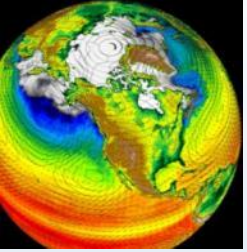
Integrated Hydro-Terrestrial Modeling (IHTM) Workshop
IHTM: Development of a National Capability

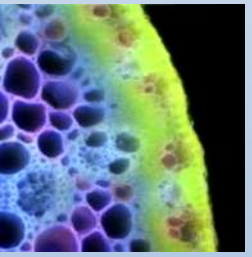
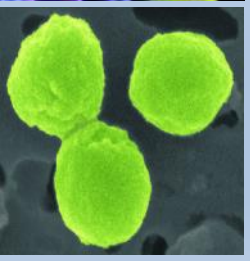
2019 IHTM Workshop

- Held September 2019 at NSF Headquarters
- Interagency leads
  - Bob Vallario (EESSD)
  - David Lesmes (USGS)
  - Tom Torgersen (former NSF)
- Co-Chairs
  - Tim Scheibe (PNNL)
  - Harry Jenter (USGS)
  - Efi Foufoula-Georgiou (UCI)
- Three “Use Cases” – Water Subcabinet
  - Water availability in the West
  - HABs, Hypoxia and Nutrient Loading
  - Flooding and Extreme Weather-Related Water Hazards
- Scheibe/Lesmes Presentation at 2019 AGU



DOE, EPA, NASA, NOAA, NSF, USACE, USBR, USDA, USGCRP, USGS



Questions?

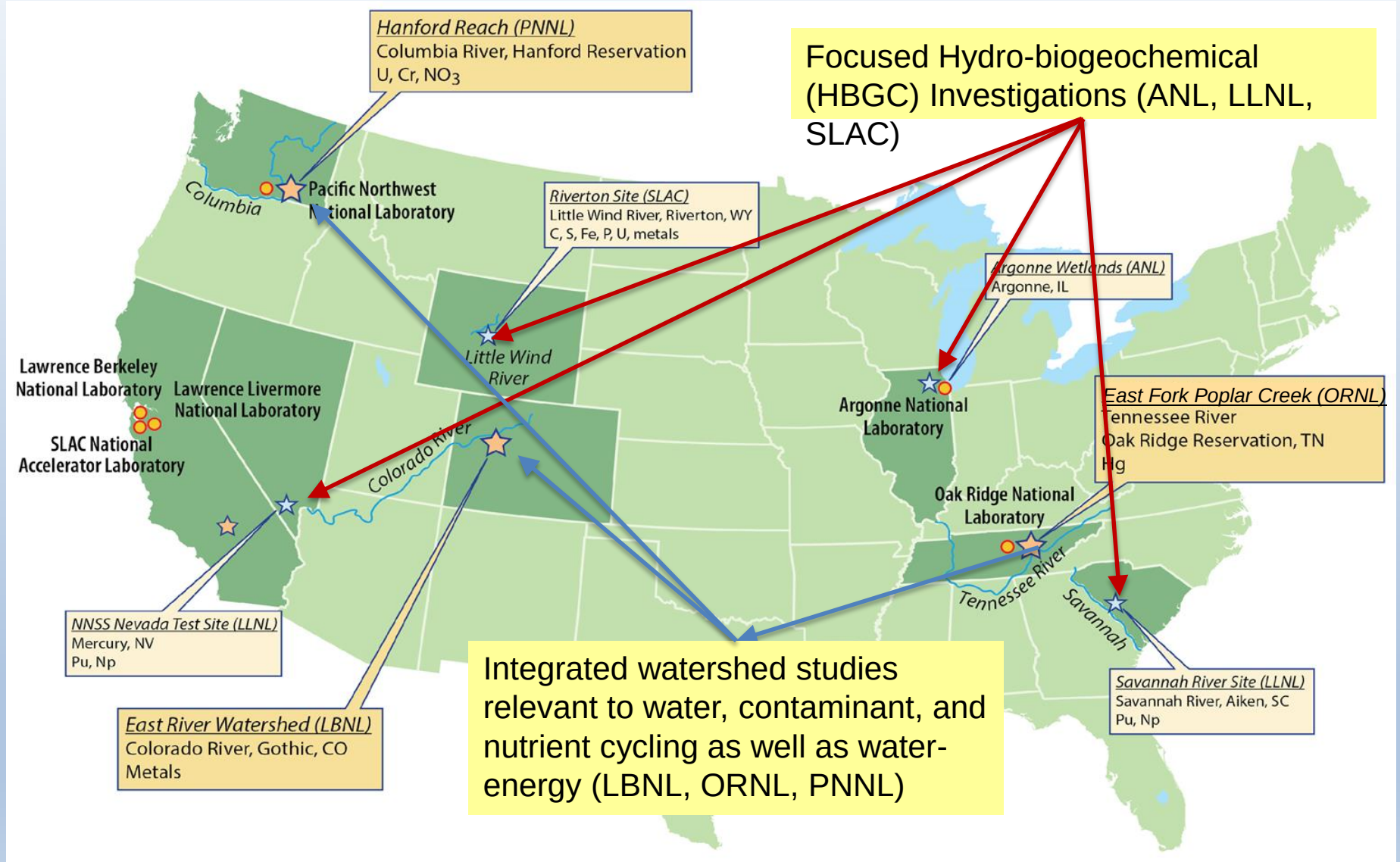
Paul Bayer, EESSD
paul.bayer@science.doe.gov

Jennifer Arrigo, EESSD
Jennifer.Arrigo@science.doe.gov

Amy Swain, BSSD
amy.swain@science.doe.gov

SBR Website: doesbr.org

SBR Network of Complementary Terrestrial Testbeds



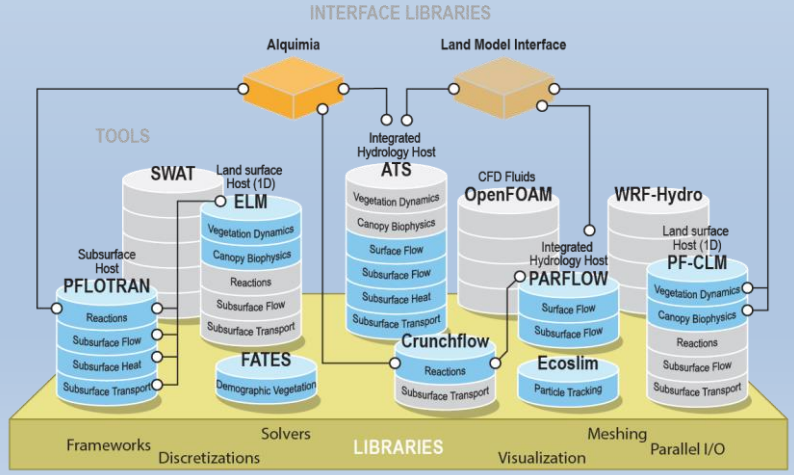
IDEAS – Watersheds Project

IDEAS – Interoperable Design of Extreme-scale Application Software

- Joint SBR/ASCR funding
- 2014-2018
- A software ecosystem of interoperable components, built on 3 SBR/TES use cases, started with “libraries”
- Spawned IDEAS-ECP, xSDK4ECP and IDEAS-Watersheds
- SW Productivity & Sustainability Plans

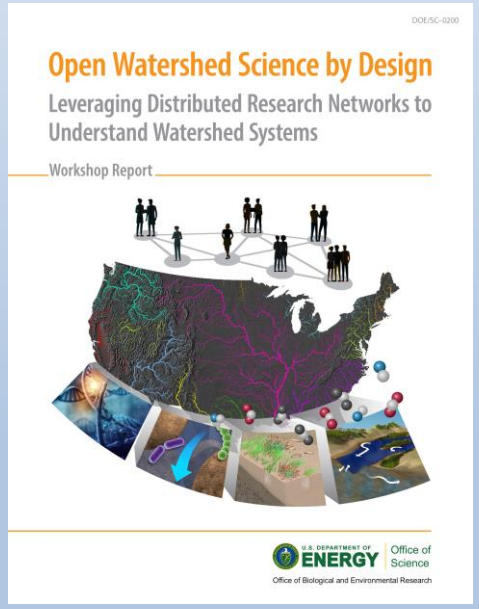
IDEAS – Watersheds

- Reviewed in 2019, 5 labs and 2 universities
- Led by D. Moulton (LANL)
- From Silos to an interoperable systems of codes/code components
- Enable integration of hydro-biogeochemical process modeling across scales
- Designed to address fragmented codes and changing HPC architectures
- Focused on specific several scales
  - Reaction-scale
  - Watershed-scale
  - CONUS-scale
  - Multi-scale
- In partnership with all 6 SBR SFAs



Open Watershed Science by Design & WHONDRS

- SBR Workshop – Jan 2019
- Leveraging Distributed Research Networks to Understand Watershed Systems
- James Stegen, Kelly Wrighton, Eoin Brodie
- In Google Docs reading file
- Presented at the Spring 2019 BERAC meeting & 2019 AGU
- Recommendations
  - Promoting FAIR data principles
  - Introduced ICON data principles
    - Integrated
    - Coordinated
    - Open
    - Networked
- Combines open science data principles with design thinking techniques
- Five use cases to do together what is not possible alone
  - WHONDRS example
  - Reaction-scale
  - Watershed-scale
  - Basin-scale
  - Multi-scale

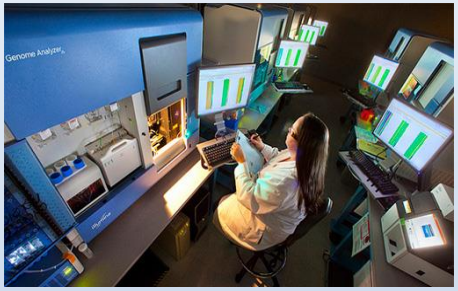


WHONDRS
Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems

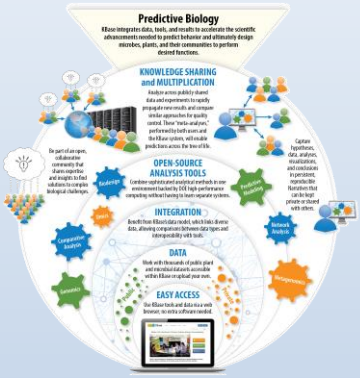
BER User Facilities/Community Resources

EMSL, JGI, KBase

EMSL enables scientists to use multiple combinations of premier experimental and modeling capabilities to obtain a mechanistic understanding of physical, chemical, and intra- and inter-cellular processes and interactions.



JGI provides genome sequencing, genome data acquisition, and genome analyses in support of DOE mission needs in bioenergy, carbon cycling and biosequestration, and biogeochemical processes.



KBase (Systems Biology Knowledgebase) is a large-scale bioinformatics system that enables users to upload their own data, analyze it (along with collaborator and public data), build increasingly realistic models, and share and publish their workflows and conclusions.

FICUS
Facilities Integrating Collaborations for User Science

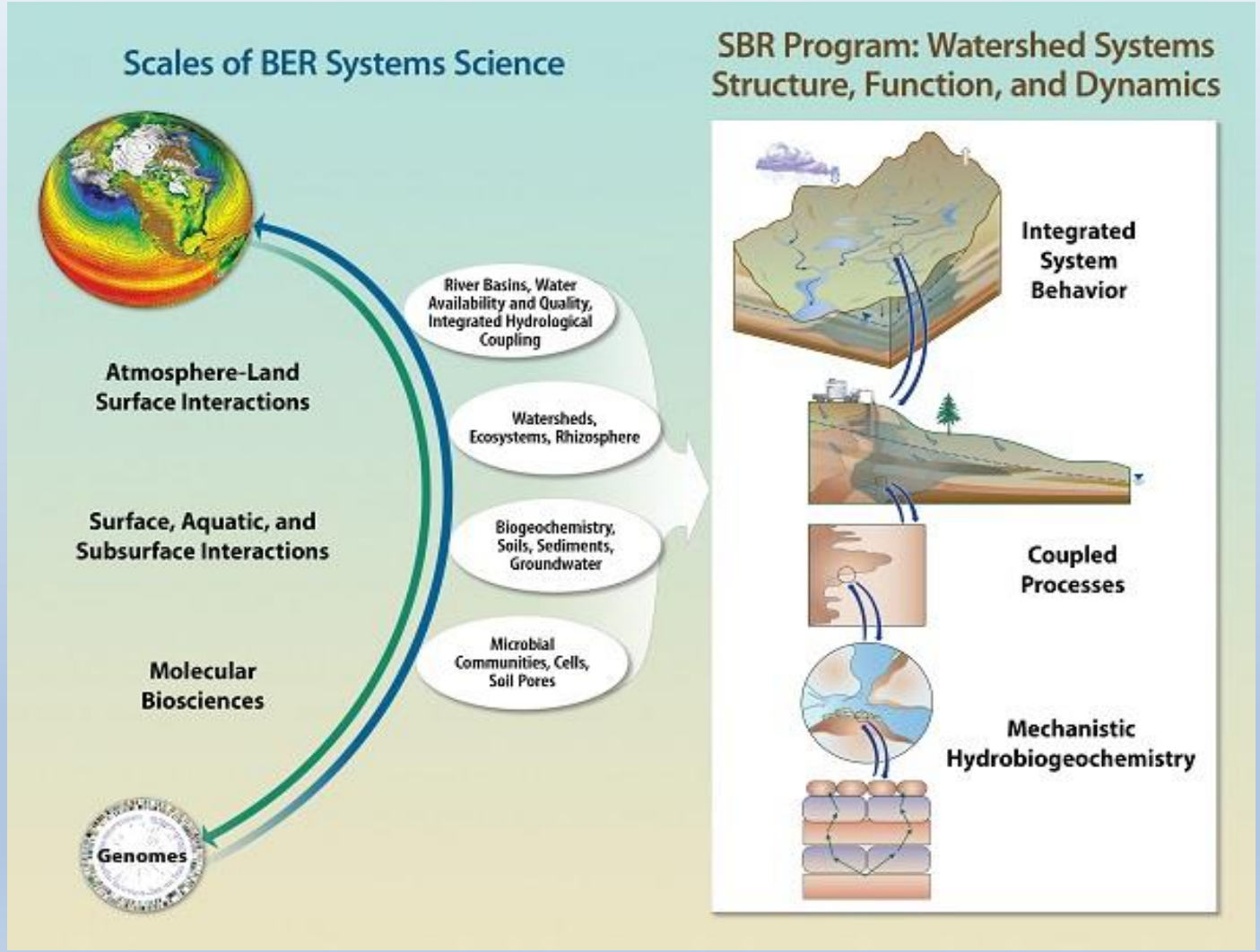
FICUS is a mechanism that enables scientists to access two Office of Science User Facilities via a single proposal (e.g., EMSL and JGI).

- See BERStructuralBioPortal.org

BER supports capabilities at the DOE synchrotron and neutron User Facilities. Free access is available for molecular- through tissue-level spectroscopic, scattering and imaging capabilities.

Subsurface Biogeochemical Research (SBR) Program

Predictive understanding of how watersheds function as integrated hydro-biogeochemical systems and how they respond to perturbations.



SBR Program: *Watershed System Science for Energy*

Scientific Understanding Enables U.S. Water and Energy Security

Addressing DOE and National Needs in:

- Contaminant management
- Clean water availability
- Safe storage of energy and nuclear byproducts in the subsurface
- Nutrient availability for sustainable biofuel crops
- Recovery of subsurface energy resources

Advancing a mechanistic understanding of Hydro-BGC that extends from plume to watershed to CONUS scales.