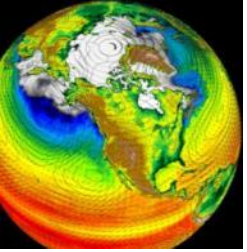
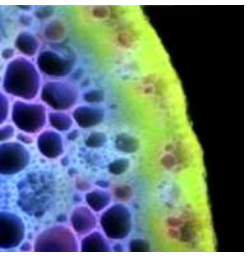
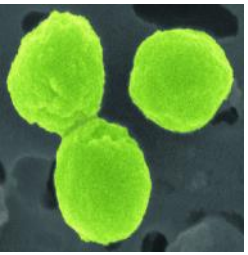


Subsurface Biogeochemical Research

SBR/TES Joint Investigators Meeting
Potomac, MD

May 1-2, 2018

David Lesmes, CESD

Paul Bayer, CESD

Amy Swain, BSSD

PI Awards and Publications

2017-2018

Geochemical Society Fellows
J. Davis (LBNL)
S. Fendorf (Stanford)
P. Santschi (Texas A&M)

AGU Fellows
S. Hubbard (LBNL) – 2017

Corporate Fellow
B. Gu (ORNL) – 2017

V.M Goldschmidt Medal
J. Banfield (UC Berkeley) – 2017

Discover Magazine – Top100 Stories
J. Banfield – Discovery of Previously Unknown Species

- 112 publications in 2015
- 120 publications in 2016
- 117 publications in 2017
- 36 publications (so far) in 2018

SBR Solicitations

- **ESS/SBR University Solicitations**
  - Scope: Within CONUS and complementary to SFAs
  - FY16 ESS FOA 1437: SBR made 12 awards (5 full; 7 explor.)
  - FY17 SBR FOA 1724: SBR made 7 awards (2 full; 5 explor.)
  - FY18 SBR FOA 1724: SBR to make a few more awards pending budget
- **Small Business Innovative Research (SBIR)**
  - Technologies for Characterizing and Monitoring Complex Subsurface Systems:
    - Scott Burge, Ruby Gosh, Don Nuzzio, Roelof Versteeg
  - SC-Wide Crosscut: Big Data Technologies for Science and Engineering
    - FY18 ASCR, BER-CESD, BER-BSSD, BES-Facilities (6 awards for BER)
    - FY19 ASCR, BER-CESD, BER-BSSD, EMSL, BES-CompChem, BES-Facilities,
    - FY19 Shared Ecosystem Requirements driven by specific use-cases: CompChem+CompBio+CompEnv+BER/BES Facilities

---

- **BER Early Career Solicitation: Lab and University Awards**
  - Previous SBR Awardees: Matt Marshall (PNNL), Helen Hsu-Kim (Duke), **Ming Ye (FSU); Joel Rowland (LANL), Jonathan Raff (Indiana U.)**

SC Graduate Student Research (SCGSR) Program

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

2018 Solicitation 1: Due May 15, 2018

Supplemental Awards. 3 to 12 months conducting part of their doctoral thesis/dissertation research at a DOE lab. Collaborate with a DOE laboratory scientist.

Environmental System Science - SBR

FY17, Round 1 (SBR)

D. Adhikari, U Nevada-Reno (N. Hess, EMSL) – Coupled biogeochemical fate of iron and iron-bound organic carbon in redox reactions.

C. Dewey, Stanford (P. Nico, LBNL) – Heavy metals and soil organic matter: complexation in cyclic redox environments.

N. Jemison, UIUC (S. Braun, LBNL) – Distinguishing U geochemical processes: an isotope approach.

FY17, Round 2 (SBR)

G. Rue, U Colorado Boulder (M. Tfaily, EMSL) – Rare Earth Elements and organometallic interactions in the aquatic environment

V.A. Rivera, Northwestern U (P. Beckman, ANL) – Data Fusion and Machine Learning for Analysis of Soil Saturation in Urban Landscapes

SBR Visioning Workshop: 2017 PI Meeting

Goal: Identify Priority Research Objectives to Drive SBR Science and Advance DOE Energy and Environmental Missions

Tuesday Evening (6:30 - 8:00 pm, Ben Franklin Hall)

6:30 pm SBR overview and expectations for Town Hall and Breakouts (D. Lesmes)

6:40 pm SBR Science: Bridging Scales and Disciplines to Advance Understanding and Enable Solutions to DOE's Energy and Environmental Challenges (S. Hubbard, T. Scheibe)

6:55 pm Overview of Watershed Systems Breakout (K. Williams)

7:05 pm Overview of Hydro-Biogeochemical (HBGC) Processes Breakout (J. Bargar)

7:15 pm Guided Discussion (S. Hubbard, T. Scheibe)

8:00 pm Adjourn

Wednesday Morning (8:30 am – 12:00 pm, Room 4 and Room 17A/B)

"Watershed Systems" Breakout (Room 4)

Hydro-Biogeochemical Processes Breakout (Room 17A/B)

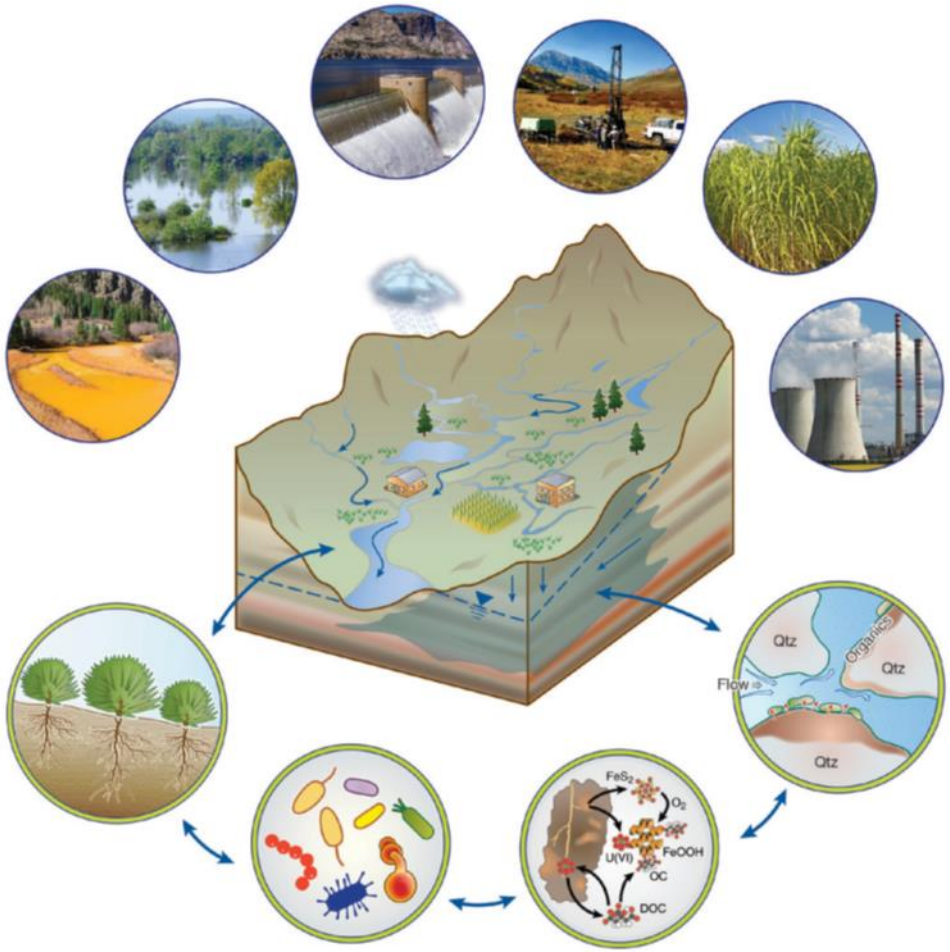
Wednesday Afternoon (4:55 - 5:20 pm, Ben Franklin Hall)

Outbriefs from the SBR Town Hall

Continued Activity Throughout the Year =>Tim Scheibe Presentation 2018 PI Meeting

SBR Program: *Watershed System Science for Energy*

Scientific Understanding Enables U.S. Water and Energy Security



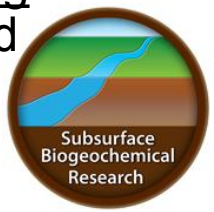
Addressing DOE and National Needs in:

- 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.

Subsurface Biogeochemical Research (SBR) Program

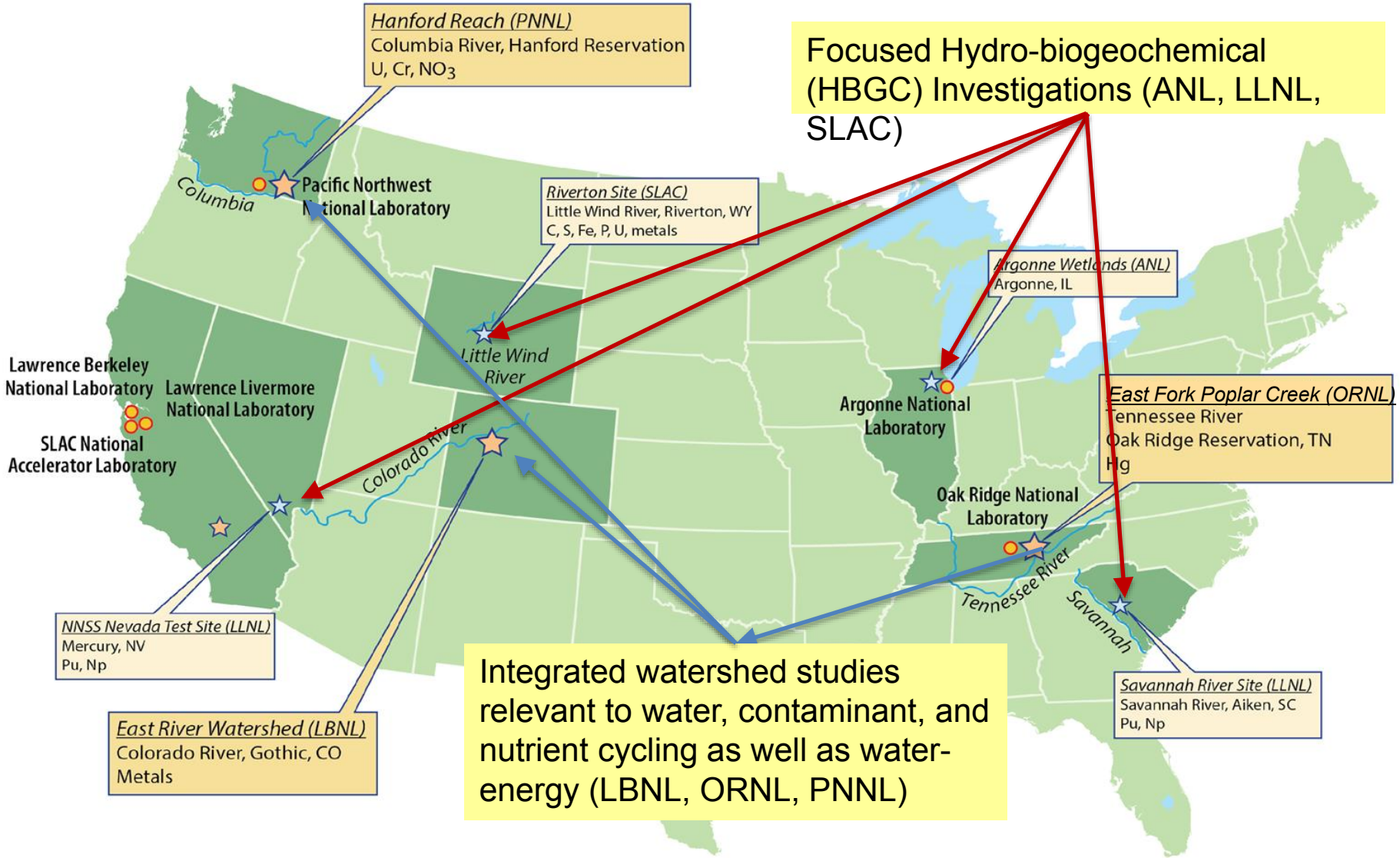
Goal: The SBR program seeks to advance a robust predictive understanding of how watersheds function as integrated hydrobiogeochemical systems and how these systems respond to perturbations.



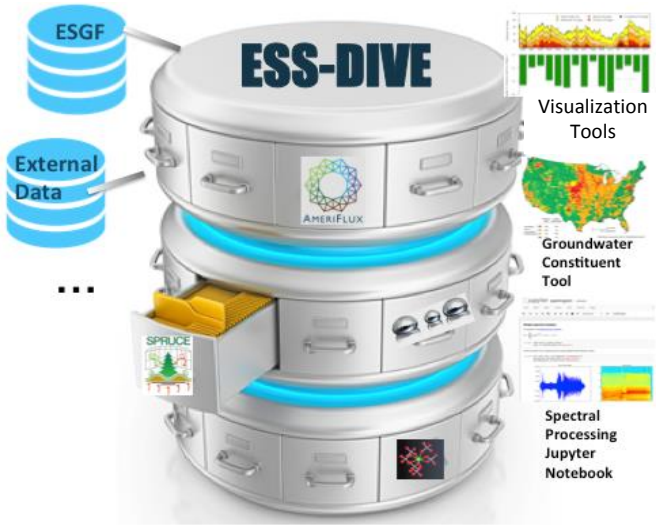
Five Priority Research Objectives:

- 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.

SBR Network of Complementary Terrestrial Testbeds



Building a Community Computational Infrastructure

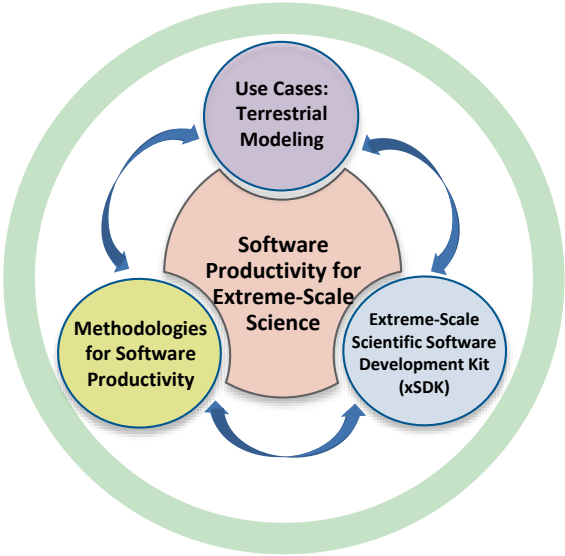


Data Management

IDEAS productivity

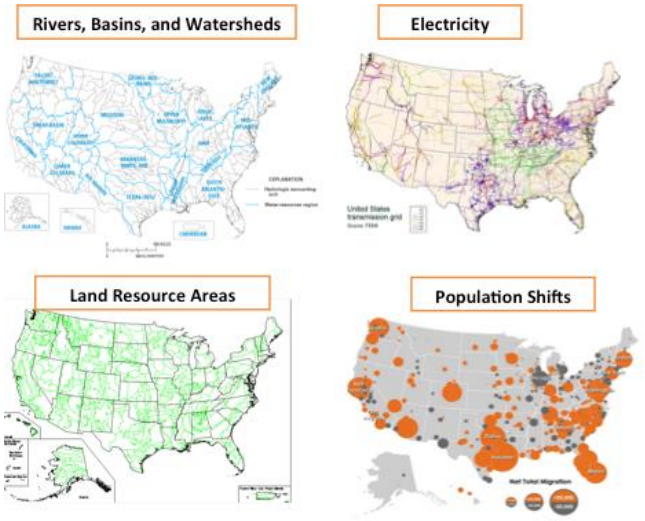
ASCR/BER

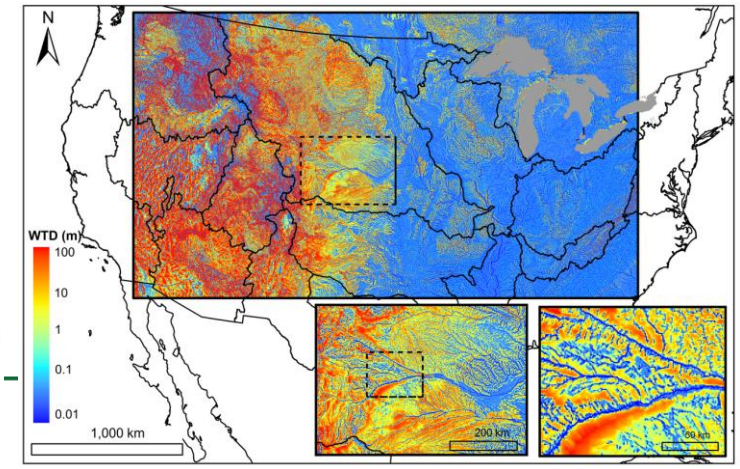
Building advanced community-based watershed system models using modern software engineering tools and methodologies that leverage DOE's Exascale Computational Investments

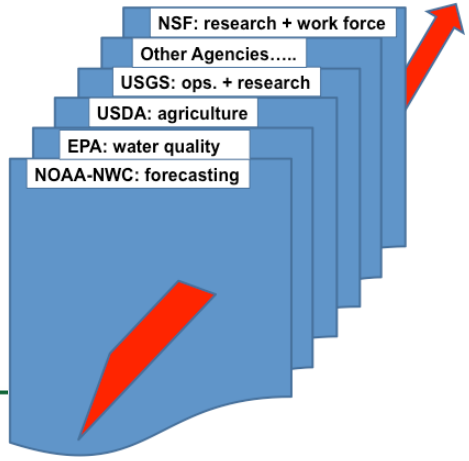


HPC model development

Connecting Across Programs and Agencies: Local ⇔ CONUS; Function ⇔ Evolution; Research ⇔ Operations

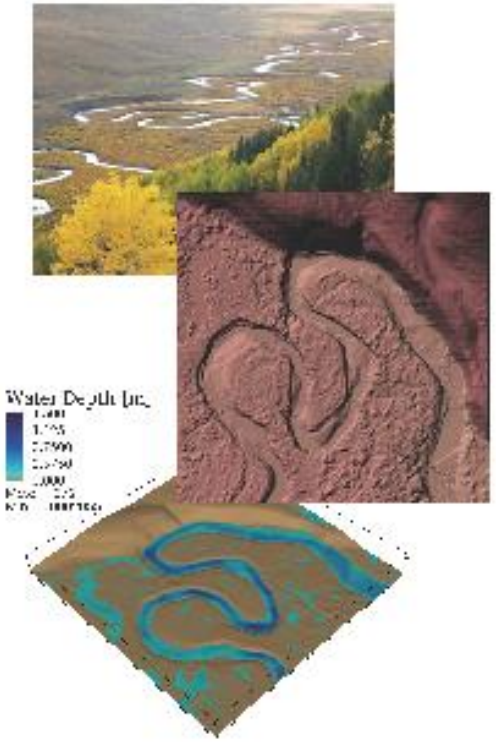




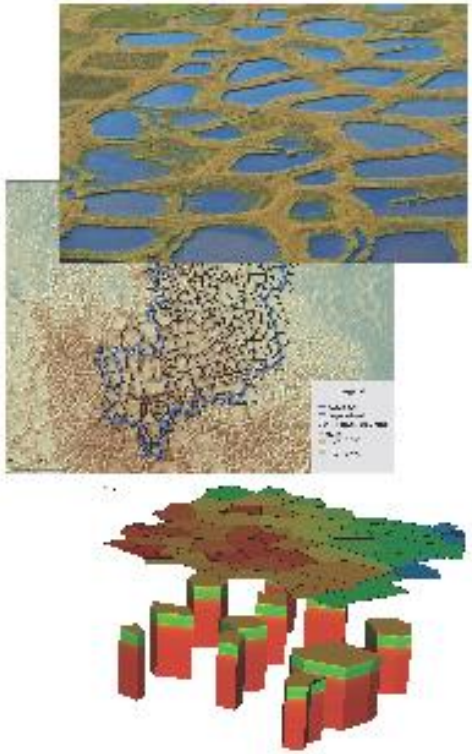


IDEAS productivity Interoperable Design of Extreme-scale Application Software (IDEAS)

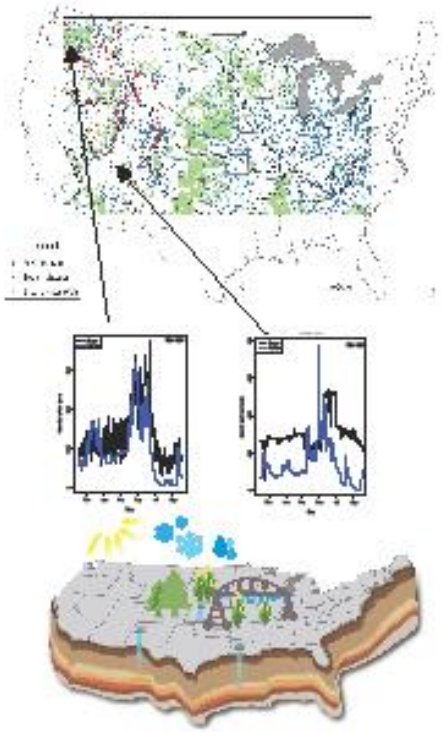
IDEAS multifaceted Use Cases use science drivers to motivate and explore software development productivity and interoperability to enhance scientific productivity.



Interoperability supports integrated hydrology studies of carbon cycling in the hyporheic zone of stream meanders at the East River watershed.

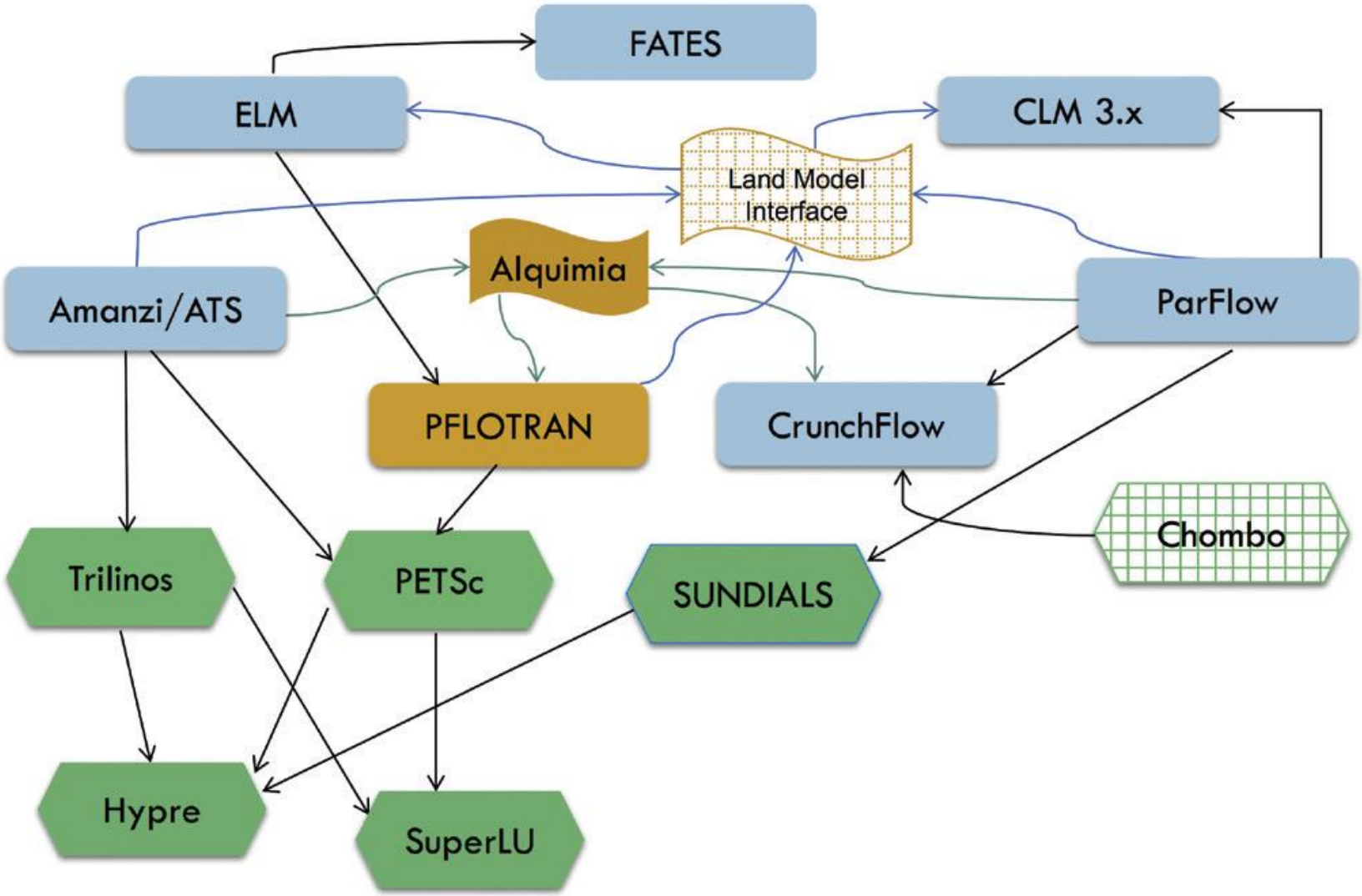


Advanced multiphysics framework and interoperable design supports process driven mixed dimensional model reduction at the Barrow Observatory

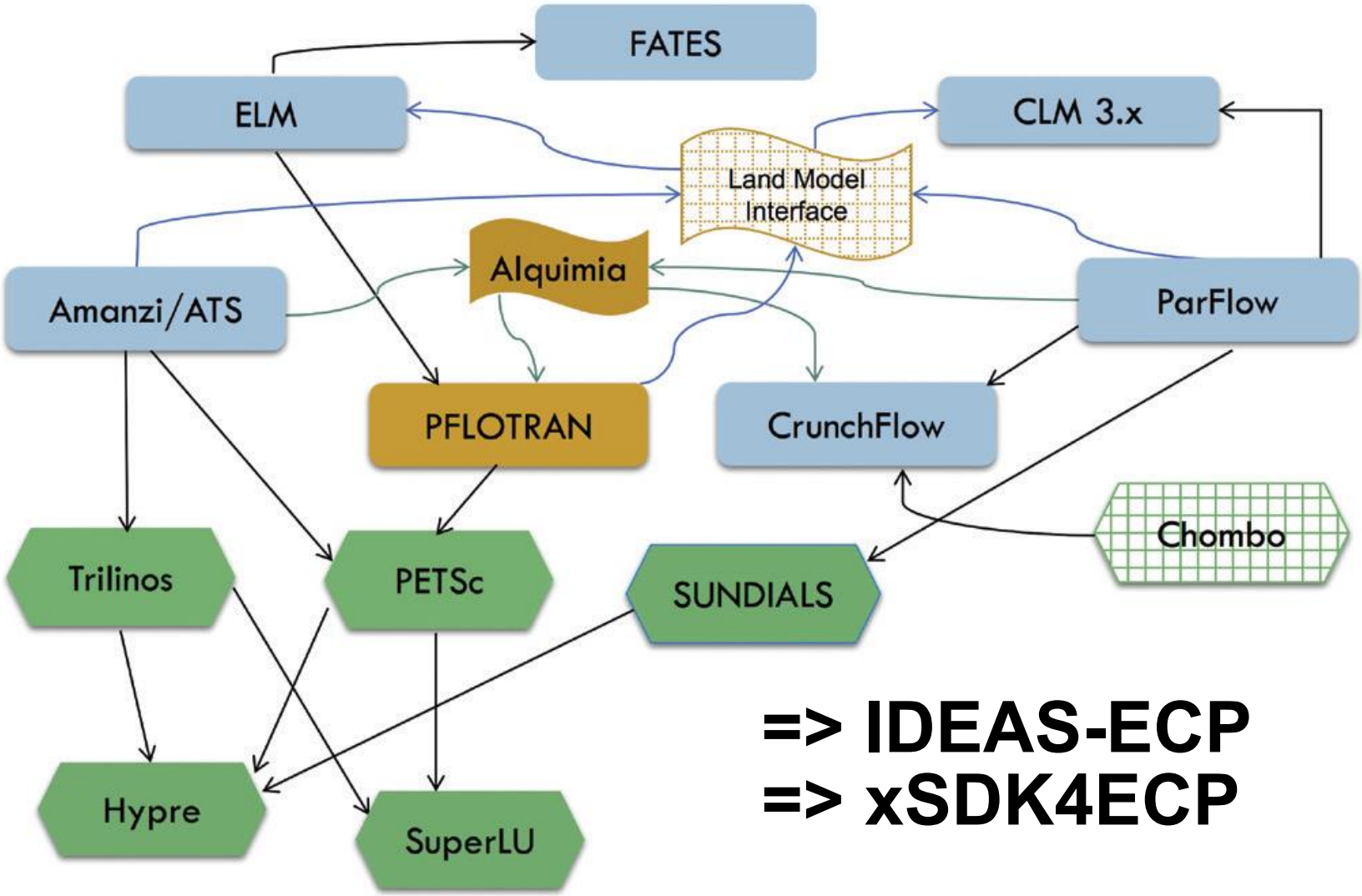


Hyperresolution simulations of integrated hydrology over the continental U.S. underpin new understanding and require scalable performance.

IDEAS : Watershed Modeling Ecosystem
(xSDK + SE Methodologies => ΔCulture)

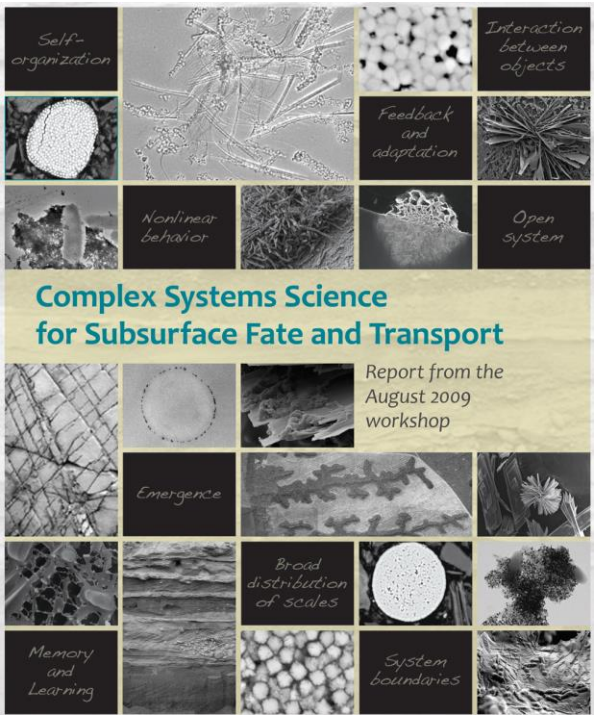


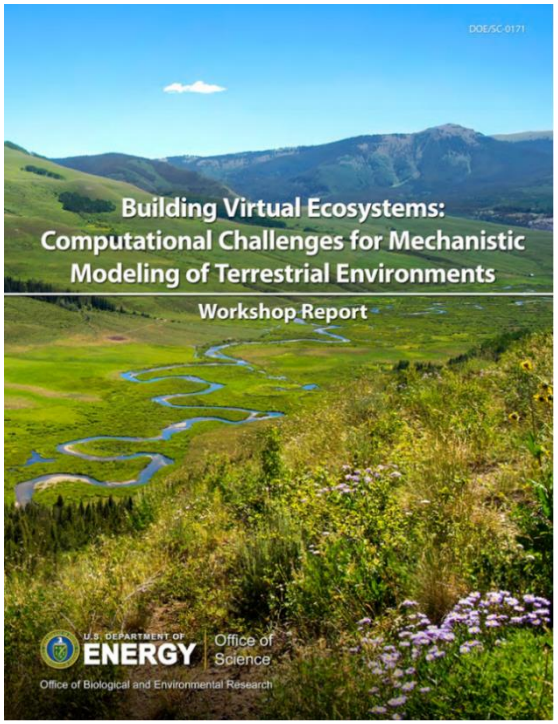
IDEAS : Watershed Modeling Ecosystem
(xSDK + SE Methodologies => ΔCulture)

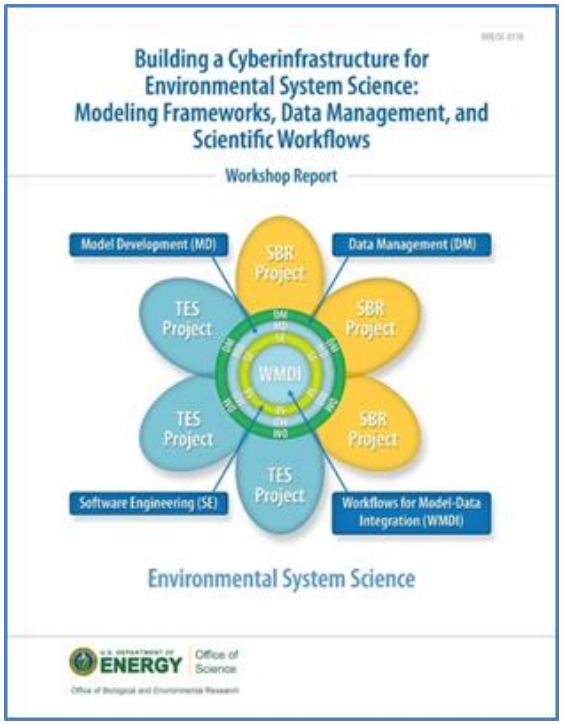


=> IDEAS-ECP
=> xSDK4ECP

Understanding Complexity and Building Capacity



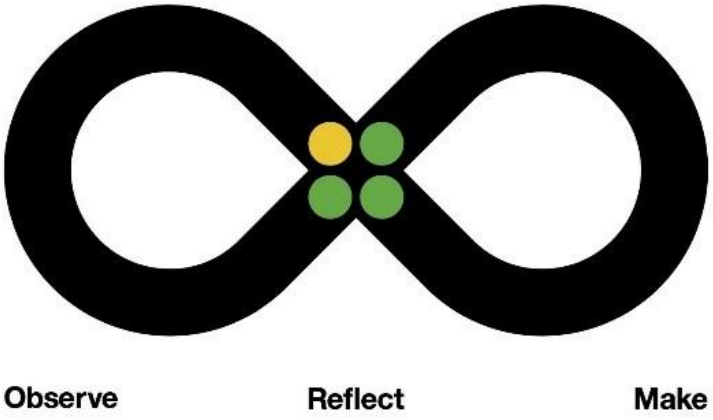




Individuals, Teams, Teams-of-Teams, Communities, Communities-of-Communities

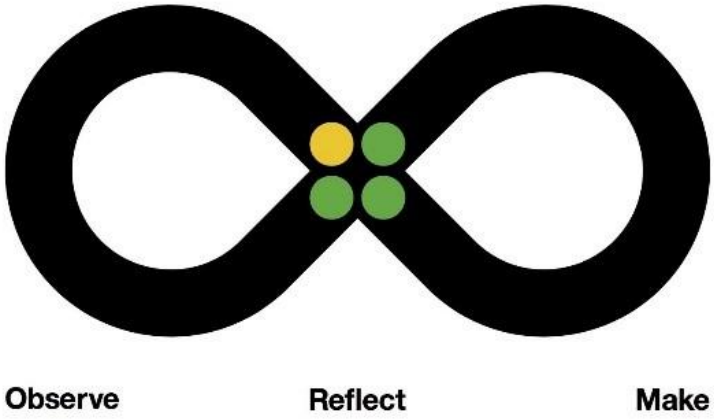
Understanding Complexity and Building Capacity

Understanding



Scientific Method

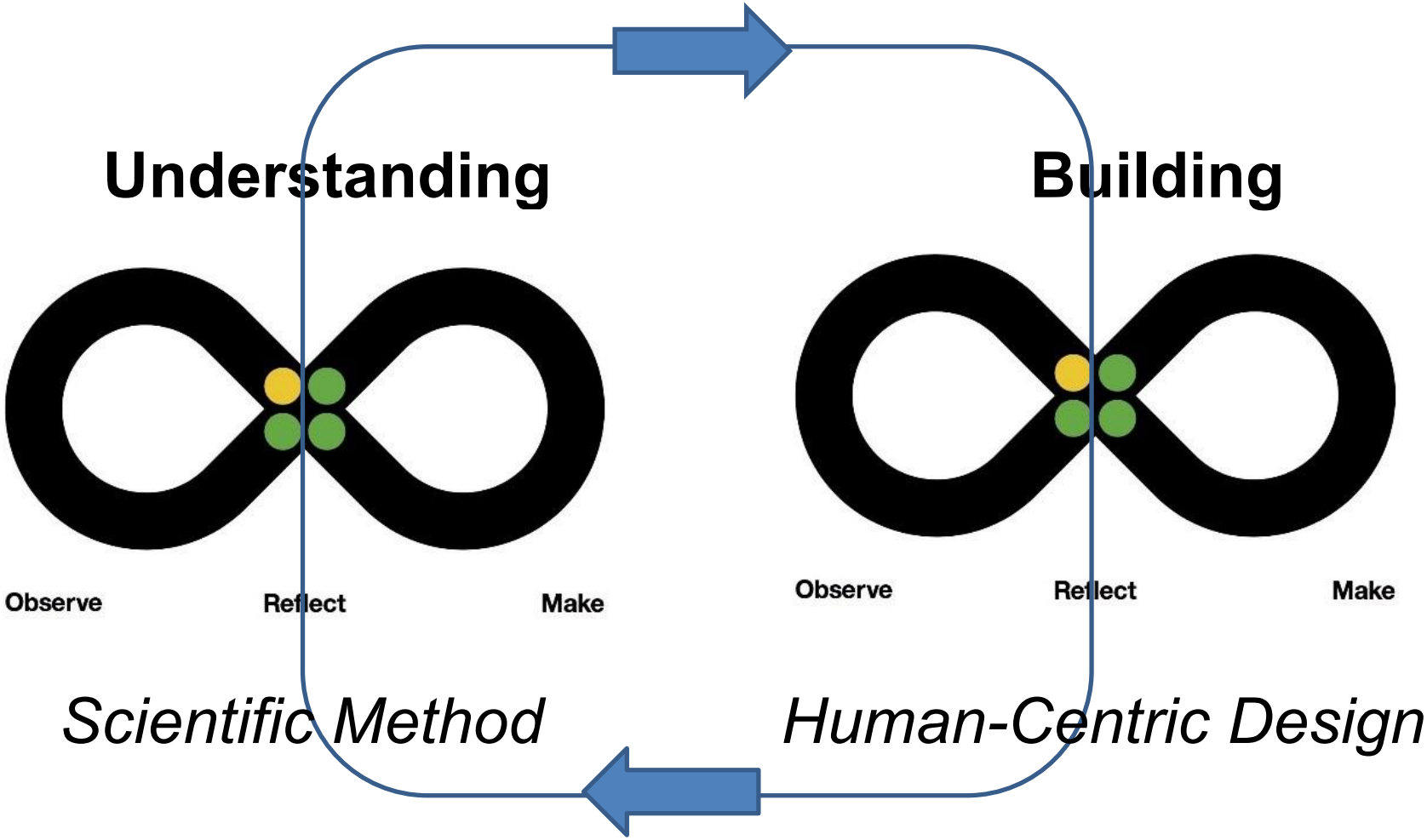
Building



Human-Centric Design

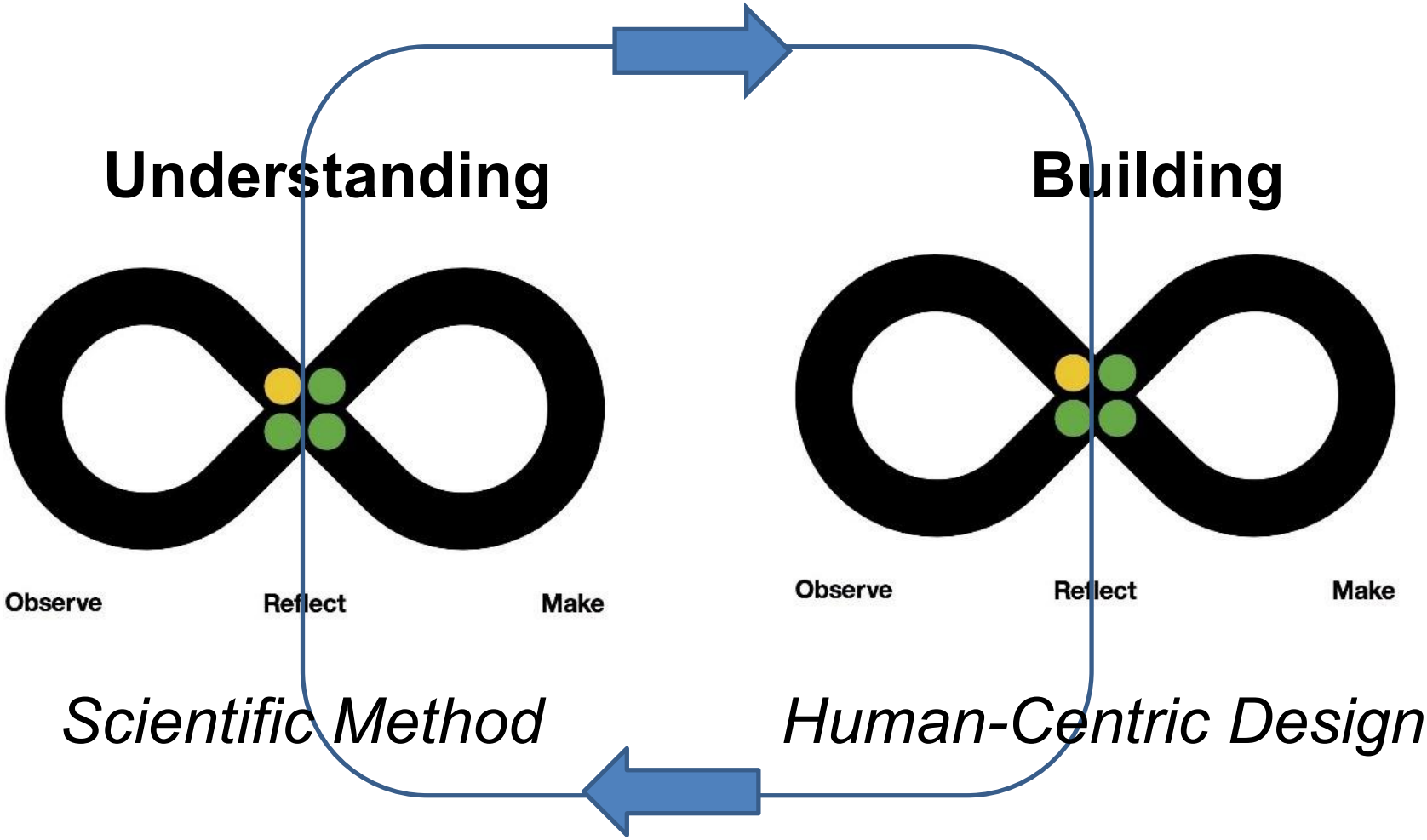
Individuals, Teams, Teams-of-Teams,
Communities, Communities-of-Communities

Understanding Complexity and Building Capacity



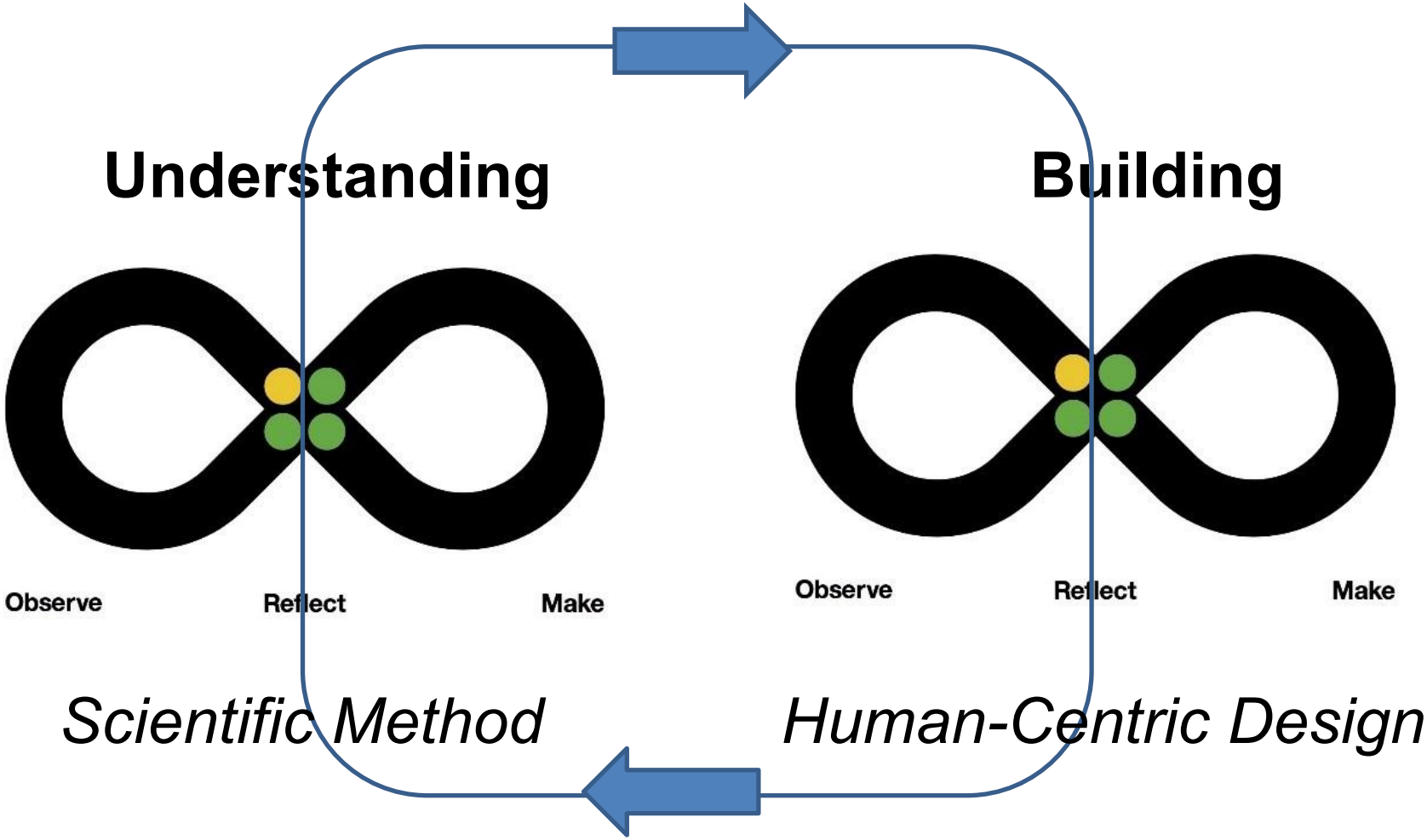
Individuals, Teams, Teams-of-Teams,
Communities, Communities-of-Communities

Understanding Complexity and Building Capacity



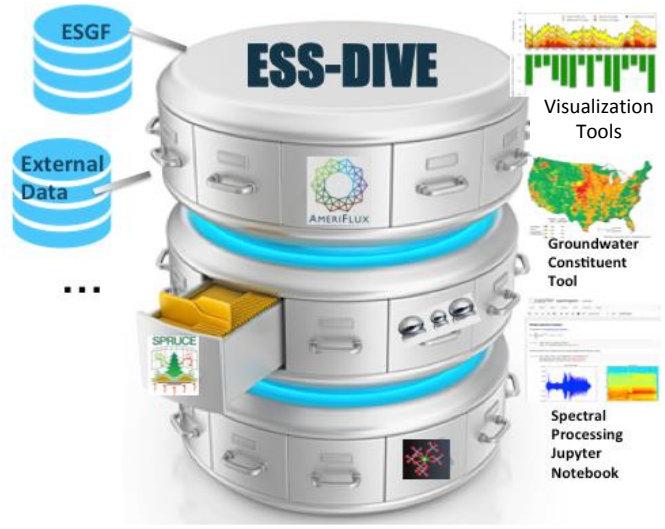
Individuals, Teams, Teams-of-Teams,
Communities, Communities-of-Communities

Understanding Complexity and Building Capacity



Individuals, Teams, Teams-of-Teams,
Communities, Communities-of-Communities

Building a Community-of-Communities Computational Infrastructure

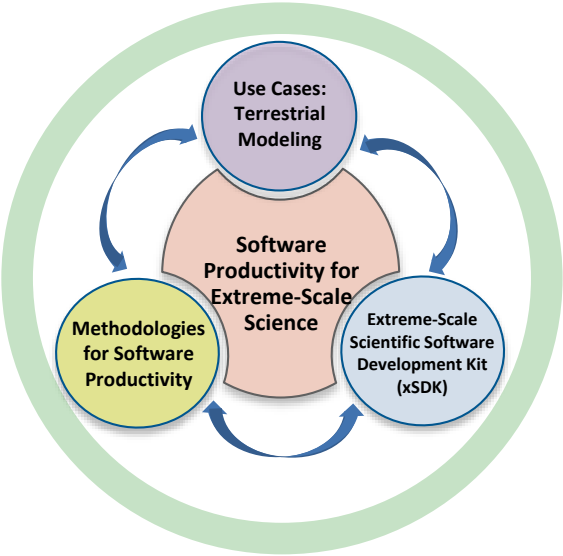


Data Management

IDEAS productivity

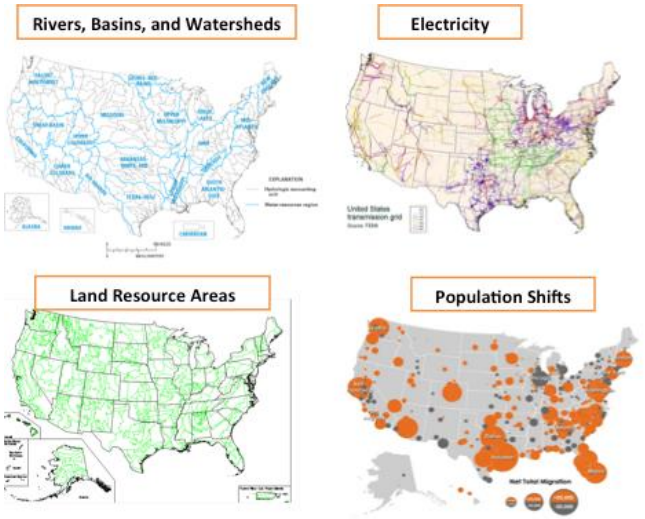
ASCR/BER

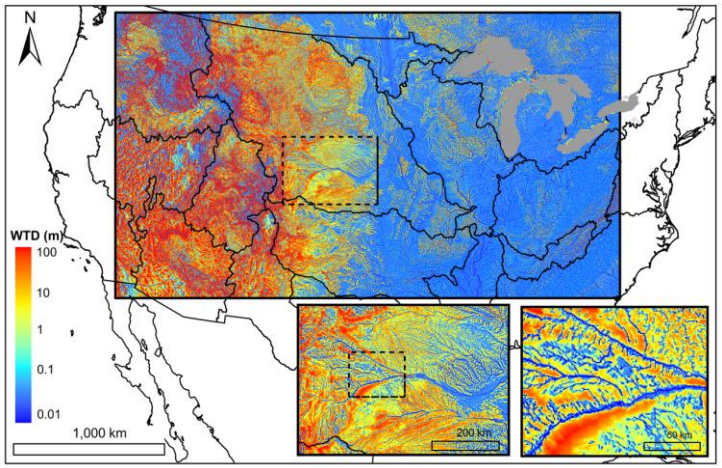
Building advanced community-based watershed system models using modern software engineering tools and methodologies that leverage DOE's Exascale Computational Investments

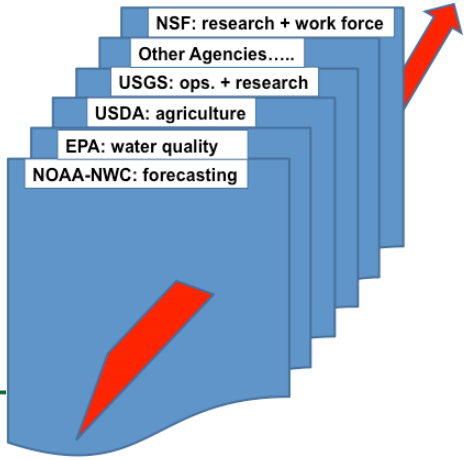


HPC model development

Convergence: Bottom-Up ⇔Top-Down + R2O2R: Technical and Social Challenges

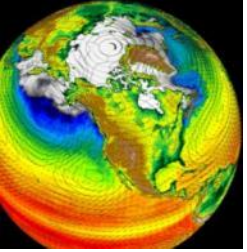


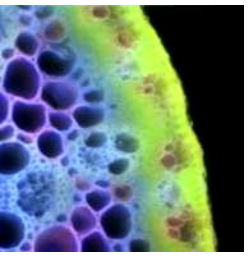
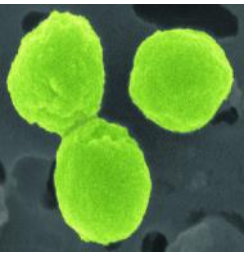




Last Thoughts….

- Lots of Interagency Discussions about Water (USGCRP, SWAQ, …)
  - Information exchange is useful, but….should bias towards action with like-minded collaborators (bilateral, multilateral, etc)
  - Set the bar low to enable initial success: focus on shared needs and synergistic capabilities
  - Start with data management challenges???
- Overcoming Fragmentation
  - "Life is seamless, but our models are not…" – Ashley Williamson, ~2013
- Developing Sustainable Business Models
  - Promote cooperation, coordination, collaboration and competition between individuals, groups, institutions, agencies and the private sector
  - To accelerate the scientific enterprise by leveraging synergies and encouraging and rewarding innovation.
- Overcoming Social Challenges Requires a Common Cause, Purpose or Belief to Motivate Collective Action
  - "*Doing Together What Would be Difficult or Impossible to Do Alone" - Accelerating Scientific Productivity and Building National Capabilities for Research and Operations*



Questions?

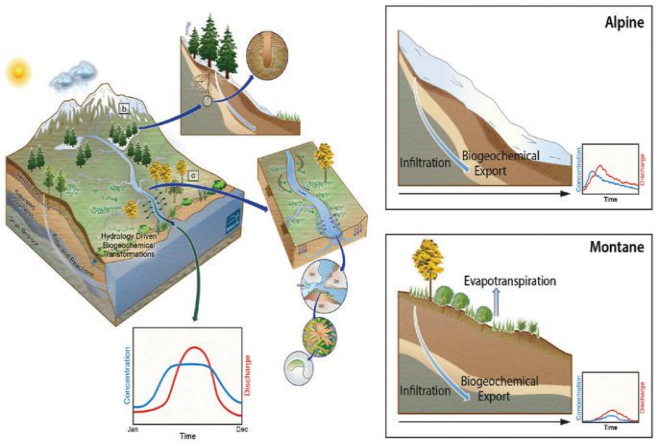
David Lesmes, CESD
david.lesmes@science.doe.gov

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

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

SBR Website: doesbr.org

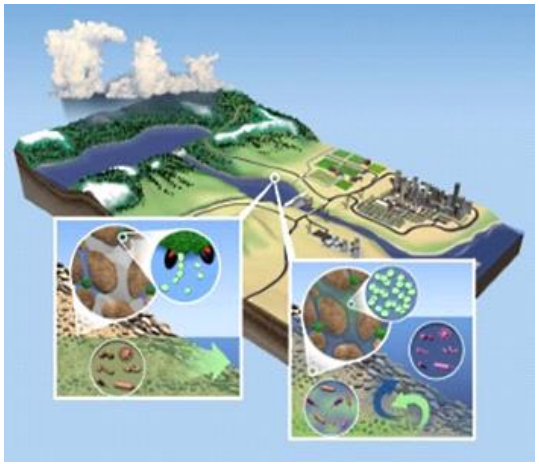
SBR Research SFAs at DOE Watershed Testbeds



LBNL SFA – **Watershed Function**

- Colorado River headwaters – heavy metals from mine tailings
- 2017 R&D 100 Award for CrunchFlow code

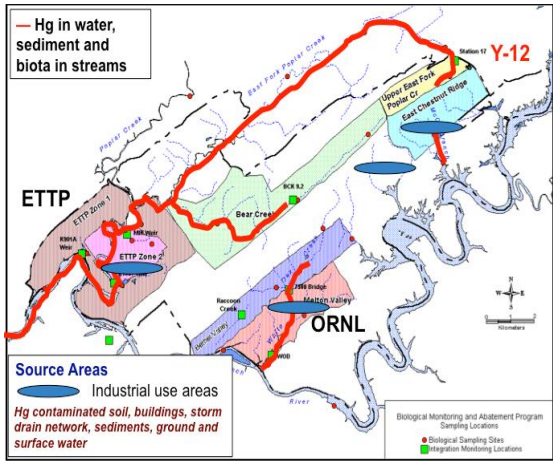
http://watershed.lbl.gov/



PNNL SFA – **Groundwater/ Surface Water Interactions**

- Columbia River, Hanford Site – U, Cr
- 2016 R&D 100 Award for Real-Time 4D subsurface imaging

https://sbrsfa.pnnl.gov/

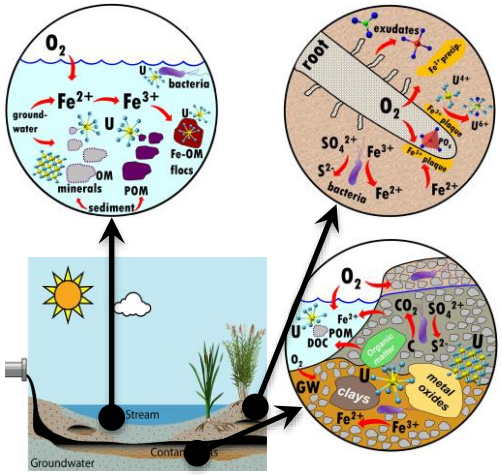


ORNL SFA – **Mercury Hydro-Biogeochemistry**

- East Fork Poplar Creek, Oak Ridge – Hg
- Discovered genes for Hg methylation

https://www.esd.ornl.gov/programs/rsfa/index.shtml

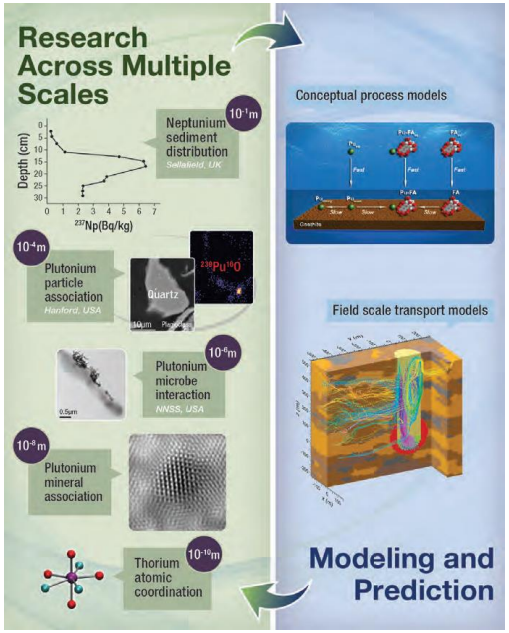
SBR Research SFAs at DOE Watershed Testbeds



ANL SFA - **Wetland Hydro-Biogeochemistry**

- Steeds Pond, Savannah River Site – U

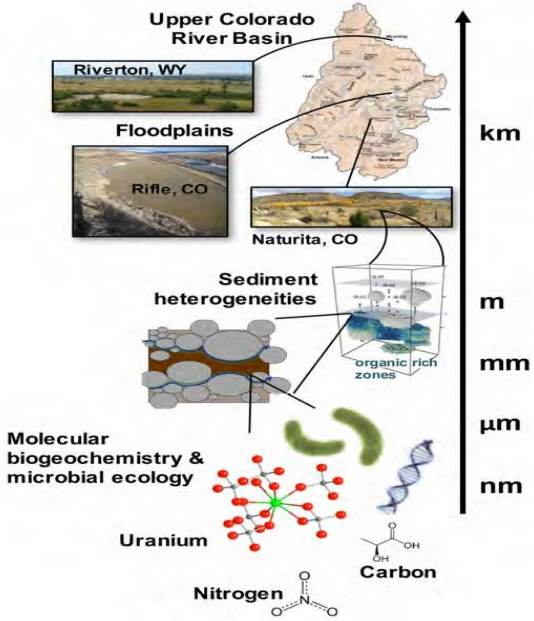
https://www.anl.gov/bio/project/subsurface-biogeochemical-research



LLNL SFA – **Actinide Biogeochemistry**

- Nevada Test Site, Hanford Savannah River – Pu & Np

https://seaborg.llnl.gov/research-environmental-radiochemistry.php



SLAC SFA – **Groundwater Quality**

- Riverton, Rifle, Naturita along the Colorado River – UMTRA Sites

https://www-ssrl.slac.stanford.edu//sfa/

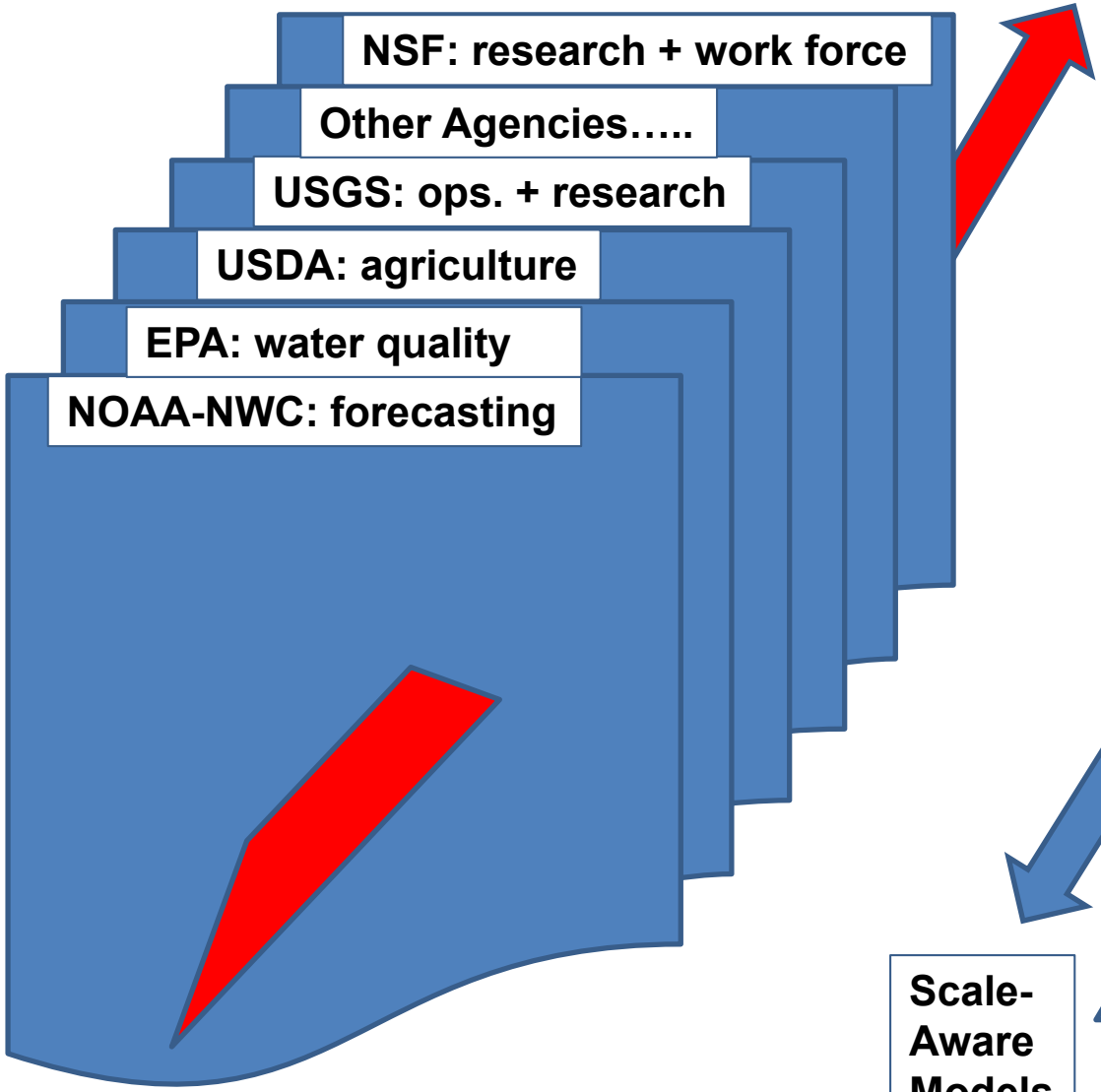
Interagency Coordination – Lots of Activity

- National Academy of Science
  - Terrestrial Modeling Discussion => Tom Torgersen (NSF)
- SWAQ
  - Terrestrial Modeling Survey/Discussion => Don Cline (USGS)
- USGCRP
  - Integrated Water Cycle Working Group => Jennifer Arrigo-Salem (USGCRP)
- Coordination with National Water Model Development
  - Community Advisory Committee for Water Prediction
  - Exploring Modes of Potential Collaboration => Webinars
- ICEMM (formerly ISCMEM)
  - Information Exchange is Useful, but….Should Bias Towards Action
  - Start with Data Management Challenges
  - Set the Bar Low to Enable Success: Focus on Shared Needs and Synergistic Capabilities
- DOE-ESS PI Meeting & CI Working Groups (April 30 - May 2, 2018)
  - Community-Based Collaborative Design Challenge (Stanford Design School)
  - Stakeholders: Dwane Young (EPA), Susan Brantley (PSU, NSF-CZOs), ….
  - Breakout Session on “Building Community Testbeds for Modeling Watershed Systems”

Classic vs Ecosystem Approaches

- **Classic application development approach:**
  - App developers write most code
  - Source code considered private
  - Make occasional use of libraries, but only those "baked into" the OS
  - Perceived low risk, **but** there are challenges (e.g., portability, maintenance)
- **Ecosystem-based application development approach:**
  - App developers use composition, write glue code & unique functionality
  - Source code includes substantial 3rd party packages
  - Risks (if 3rd party code is poor):
    - Dependent on portability of 3rd party code
    - Upgrades of 3rd party package can be disruptive (interface changes, regressions)
  - Opportunities (if 3rd party code is good):
    - 3rd party improvements and new capabilities are yours (for free!)
    - Portability to new architectures is seamless
- **Ecosystem imperative: High quality is essential, more affordable**

Integrated Water Prediction Across Scales & Communities: Shallow & Wide (operational) + Deep & Narrow (research)



DOE: Watershed Function

Deep HPC Expertise

Deep Process Understanding:

>Mechanistic: Phys+Chem+Bio

Well Characterized "Test Beds"

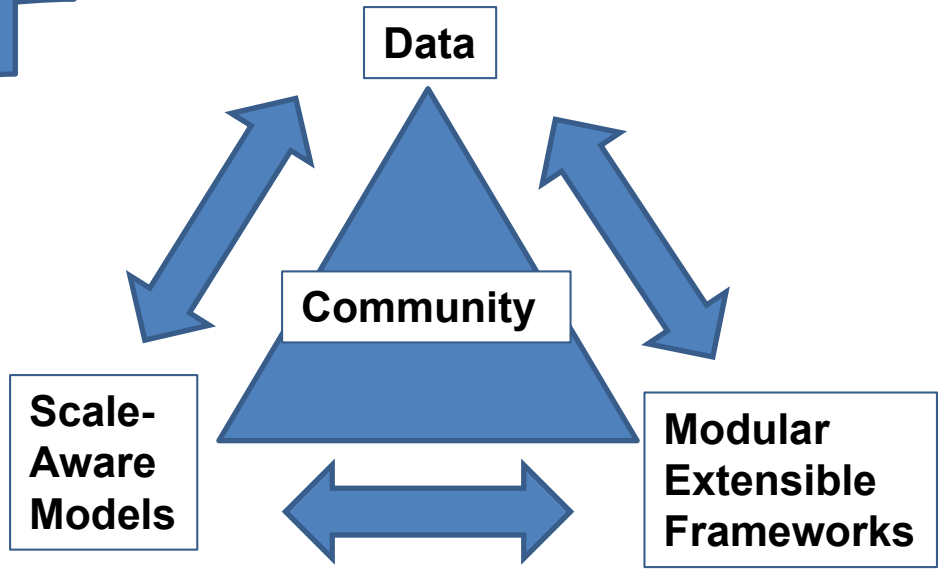
But incomplete….

>Local test beds with specific focus

>Missing system components

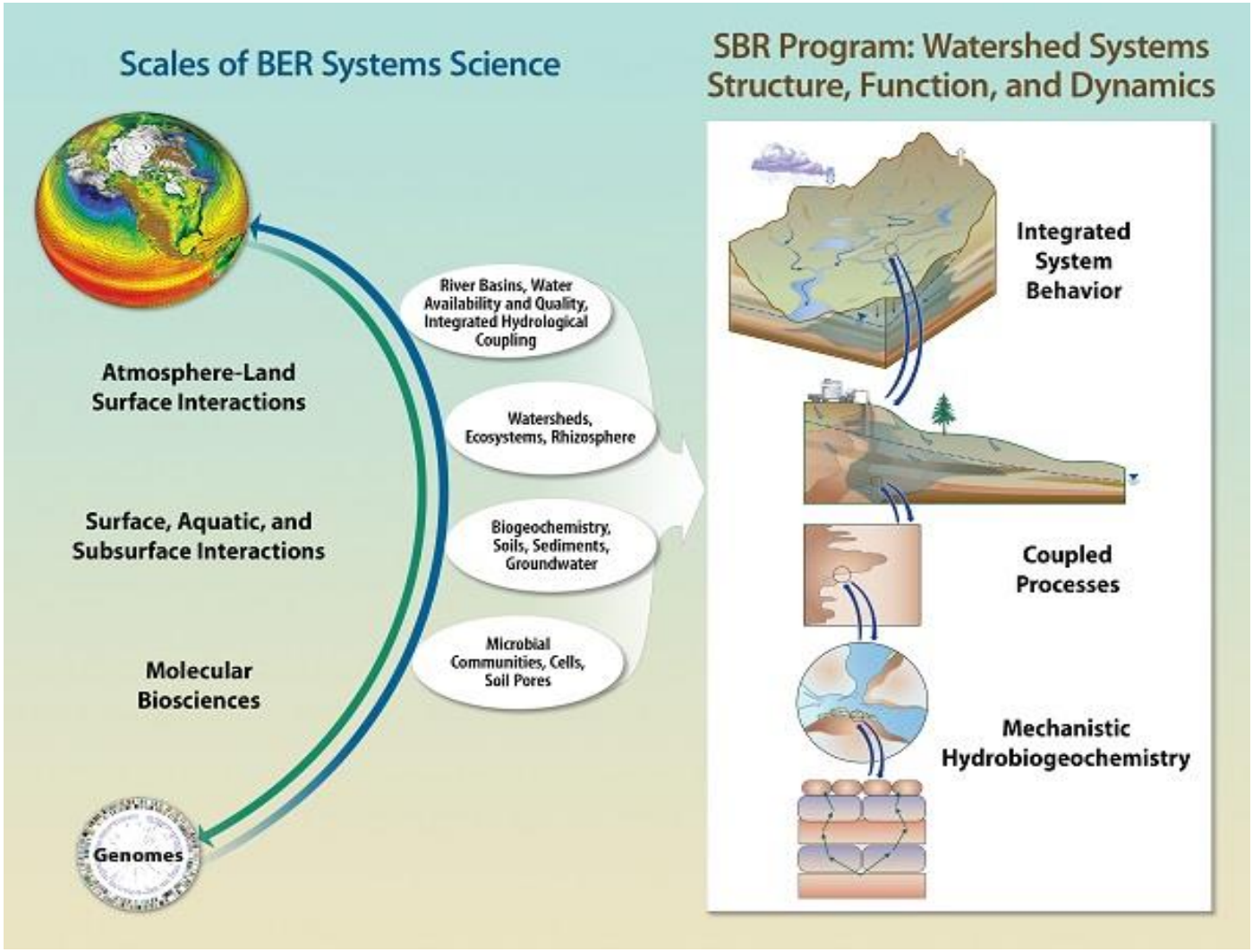
>Need data from external sources

Research + Operations = Win-Win



Subsurface Biogeochemical Research (SBR) Program

Predictive understanding of how watersheds function as integrated hydrobiogeochemical systems and how they respond to perturbations.



SBR in CESD's Strategic Planning

Vision: Improve a systems level understanding and predictability of the earth system in support of DOE's mission, through integrative theory, modeling, and experiment, over a variety of spatial and temporal scales.

Scope: Integration of atmospheric, oceanic, terrestrial, ecological, hydrological, and human components, and inclusion of system level uncertainty quantification

High level Grand Challenges

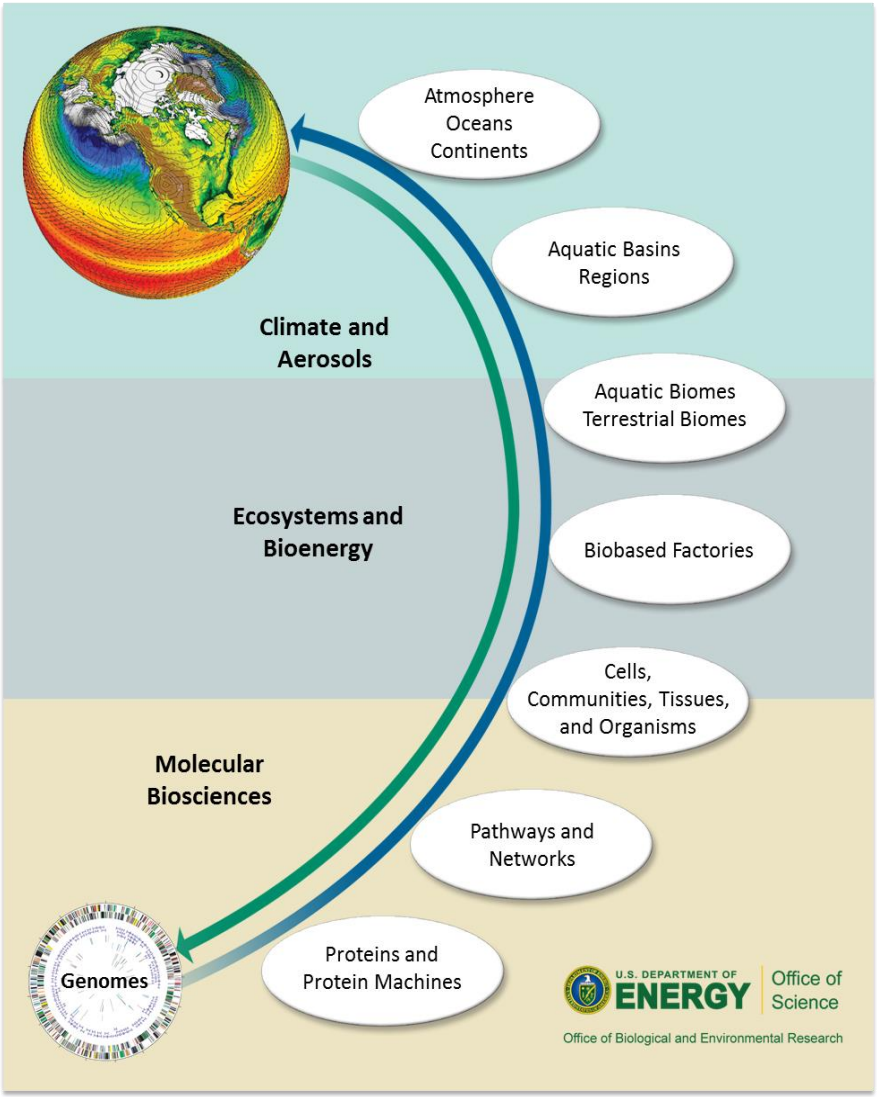
- System forcers – drivers of the coupled Earth-energy-human system.
- High latitude – process feedbacks and interdependencies with the global system.
- Biogeochemistry – biogeochemical processes and cycles across multiple scales.
- Integrated water cycle – scale aware and response to short and long-term perturbations.
- Data-model integration: interconnected capabilities and facilities that support the integration and management of models, experiments, and data across a hierarchy of scales and complexity.

SBR Science Focus Areas

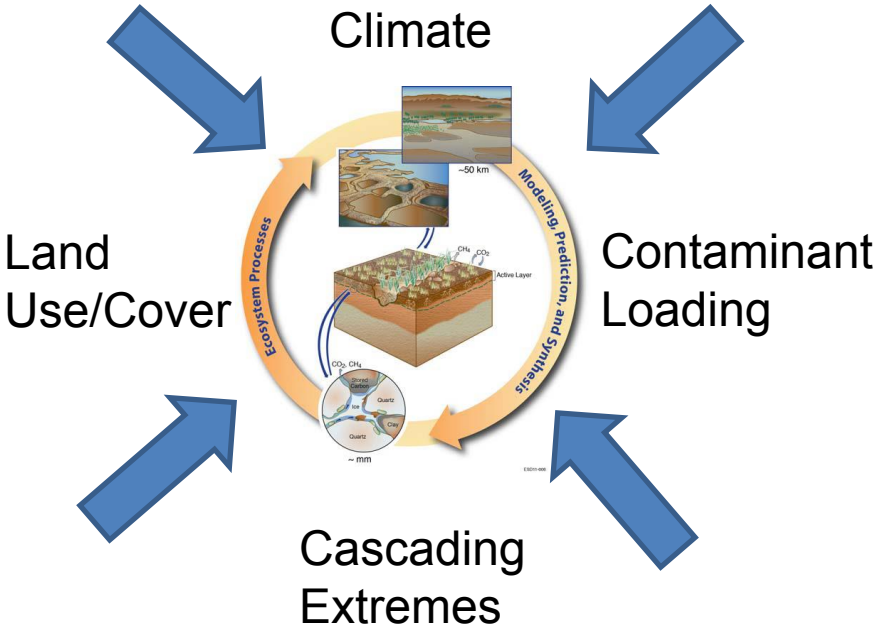
- **LBNL: Watershed Function**
  - Biogeochemical dynamics from genome to watershed scales.
- **PNNL: River Corridor and Hydro-biogeochemistry**
  - Developing a mechanistic understanding of coupled hydrologic and biogeochemical processes in large, dynamic rivers and associated watersheds.
- **ORNL: Biogeochemical Transformations at Critical Interfaces***
  - Determining the coupled hydro-biogeochemical processes controlling mercury fate and transformation in low-order freshwater stream systems.
- **ANL: Fe and S Biogeochemistry in Redox Dynamic Environments***
  - Understanding the interplay among microbial metabolic activities, solution chemistry, and mineralogy that contribute to element and contaminant transformations.
- **LLNL: Subsurface Biogeochemistry of Actinides***
  - Identifying biogeochemical processes that control actinide mobility in the environment.
- **SLAC: Groundwater Quality**
  - Investigating the coupling of fine-scale hydrologic and biogeochemical processes in transiently saturated zones.

Biological and Environmental Research

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

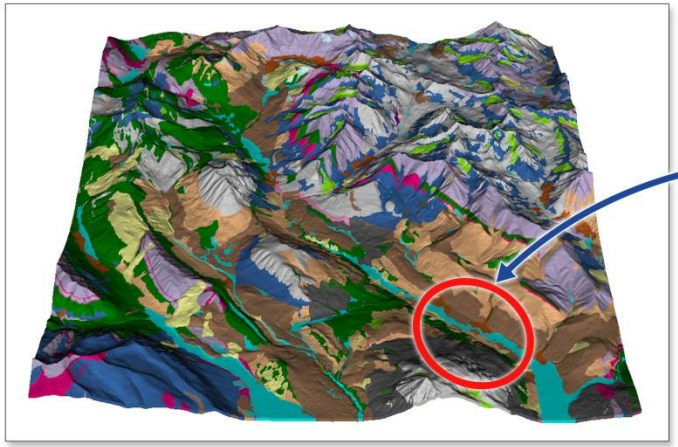


Watershed Function and Dynamics:
Mechanistic and Multiscale Understanding of Integrated System Response to Perturbations

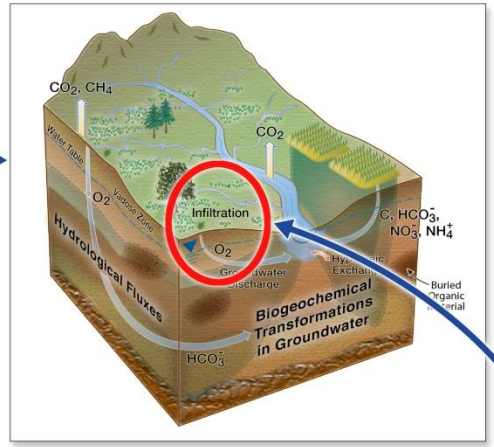


DOE Energy and Environmental Mission

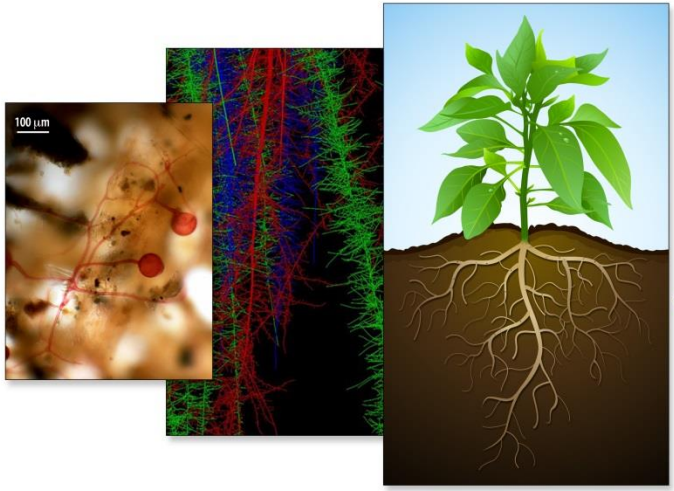
Building Virtual Ecosystems:
Virtual Plant-Soil System ⇔ Virtual Plot ⇔ Virtual Watershed



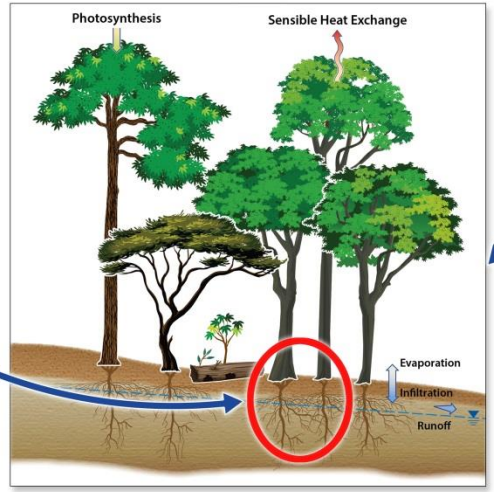
Watershed-scale processes



Catchment-scale hydrology and biogeochemistry

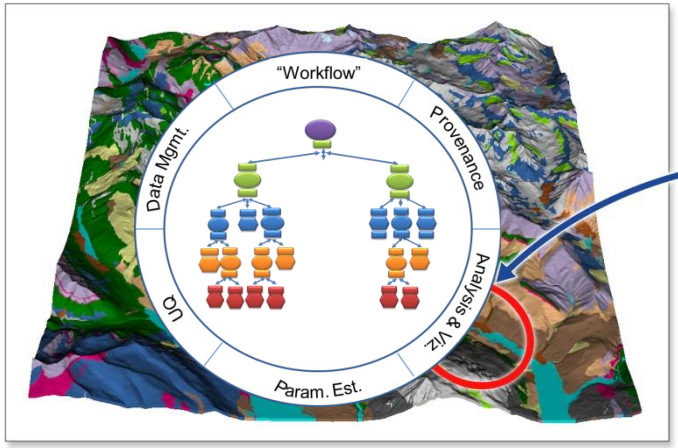


Root interactions with soil and the microbiome

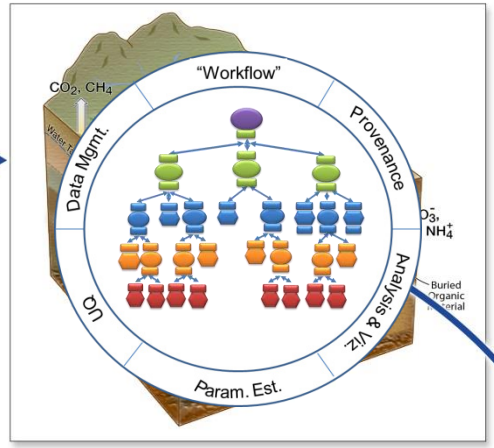


Plot-scale hydrology and vegetation

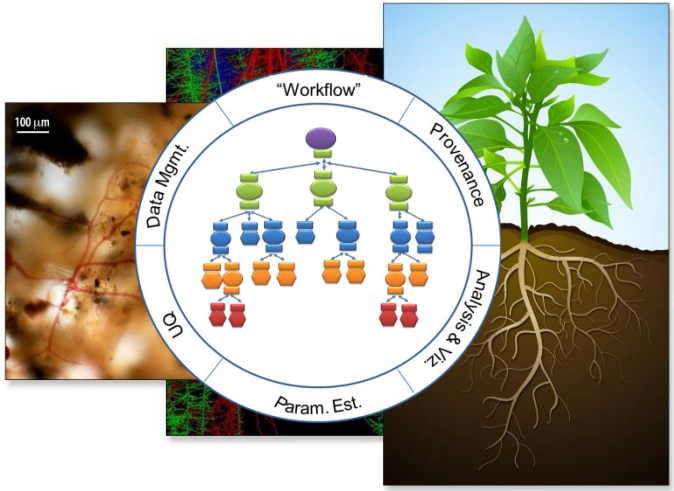
Building Virtual Ecosystems:
Virtual Plant-Soil System ⇔ Virtual Plot ⇔ Virtual Watershed



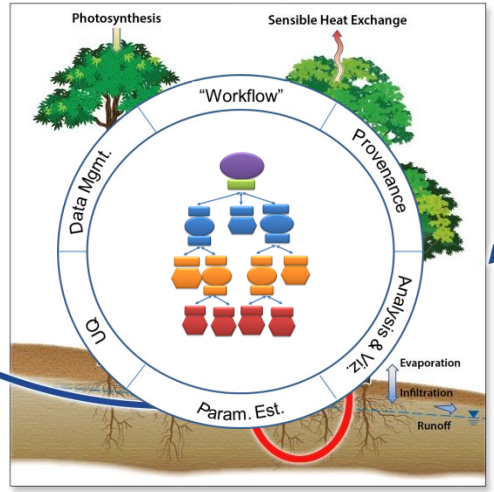
Watershed-scale processes



Catchment-scale hydrology and biogeochemistry



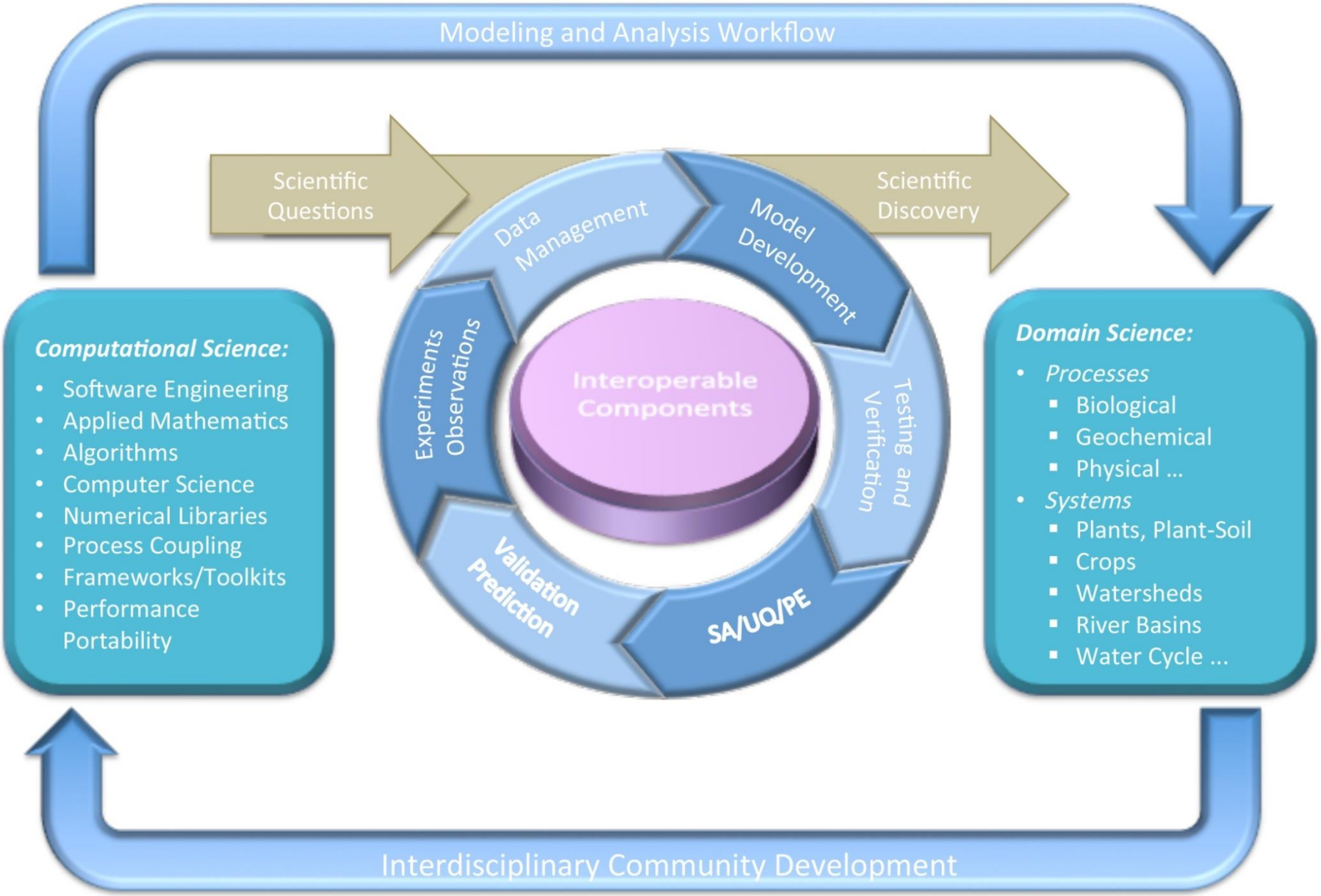
Root interactions with soil and the microbiome



Plot-scale hydrology and vegetation

Integrated Software Ecosystem

Building Virtual Ecosystems: Plants to Plots to Watersheds and Beyond…



ESS-DIVE: A New Data Archive for Earth and Environmental Science Data

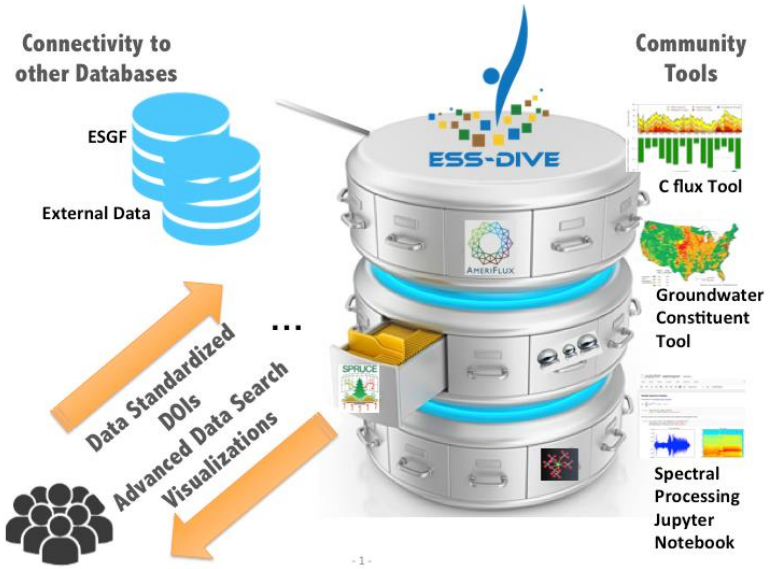
Challenge

Preserve, expand access to, and improve usability of critical data generated through DOE-sponsored research of terrestrial and subsurface ecosystems

http://ess-dive.lbl.gov

Approach and Results

- Environmental System Science - Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) available for archiving of data as of April 2018
- Leverage emerging digital library technologies and data standards
- Data citation using Digital Object Identifiers (DOI)
- Engage the community in the design of the archive
- Incentivize data providers to contribute well-structured, high-quality data
- Transition legacy DOE data into the new archive



Significance and Impact

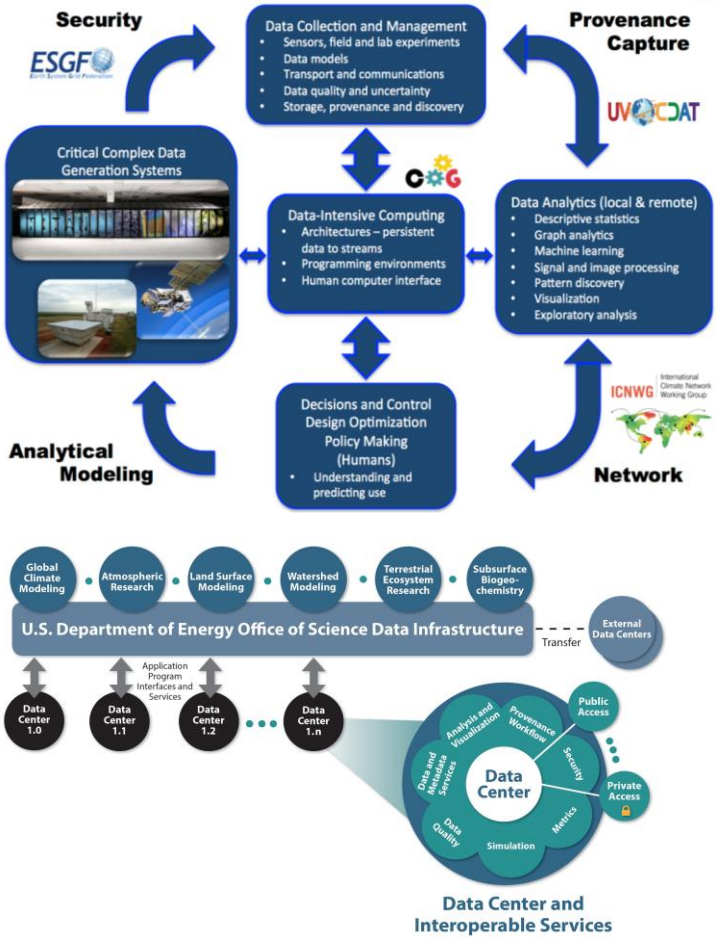
- Enables the scientific community to archive and publish critical environmental science data
- Users will be able to find and obtain data generated by ESS researchers in usable formats

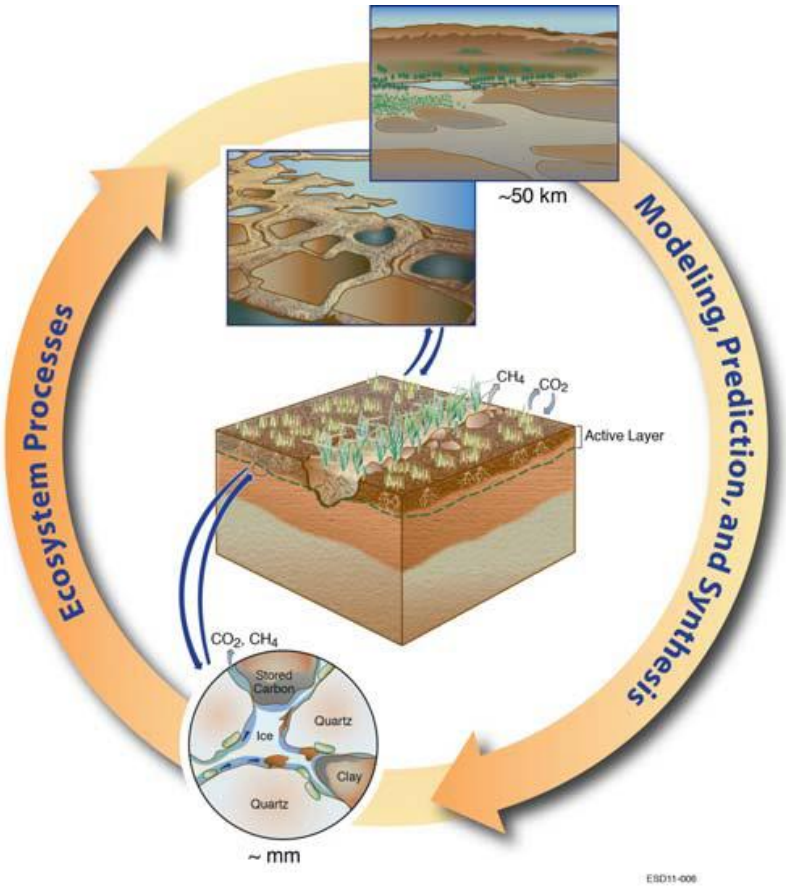
Participants:

- Lawrence Berkeley National Laboratory (LBNL)
- National Energy Research Scientific Computing Center (NERSC)
- National Center for Ecological Analysis and Synthesis (NCEAS)

Reference: D. Agarwal, C. Varadharajan, et al., IN12B-06 Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) - A New U.S. DOE Data Archive, Presented at American Geophysical Union Fall Meeting 2017.

ESS Community Cyberinfrastructure and the Virtual Laboratory





Reconciling different view points and emphasis into requirements for a new data center and a phased approach to community-based cyberinfrastructure development.

IDEAS productivity