Subsurface Biogeochemical Research

TES/SBR Joint Investigators Meeting
Potomac, MD

April 27-28, 2016

David Lesmes, CESD

Paul Bayer, CESD, EMSL

Roland Hirsch, BSSD

Thank You and Congratulations!
Recent SBR PI Award Recipients (2014-2015)

ACS Chemistry for Life®

ACS Garvan-Olin Medal
A. Kersting (LLNL) – 2016

AGU American Geophysical Union

AGU James B. Macelwane Medal
K. Maher (Stanford) - 2015

The Ernest Orlando Lawrence Award

DOE Lawrence Award winner
J. Zhou (Univ. Oklahoma) – 2014/15

American Academy of Microbiology

AAM Fellows
F. Loeffler (ORNL/UT) - 2016

UT-BATTELLE

Researcher of the Year
B. Gu (ORNL)

AAAS Advancing Science, Serving Society

AAAS Fellows
T. Barkay (Rutgers Univ.) – 2016

Australian Academy of Science

Corresponding Member
J. Banfield (Univ. of CA-Berkeley) - 2015

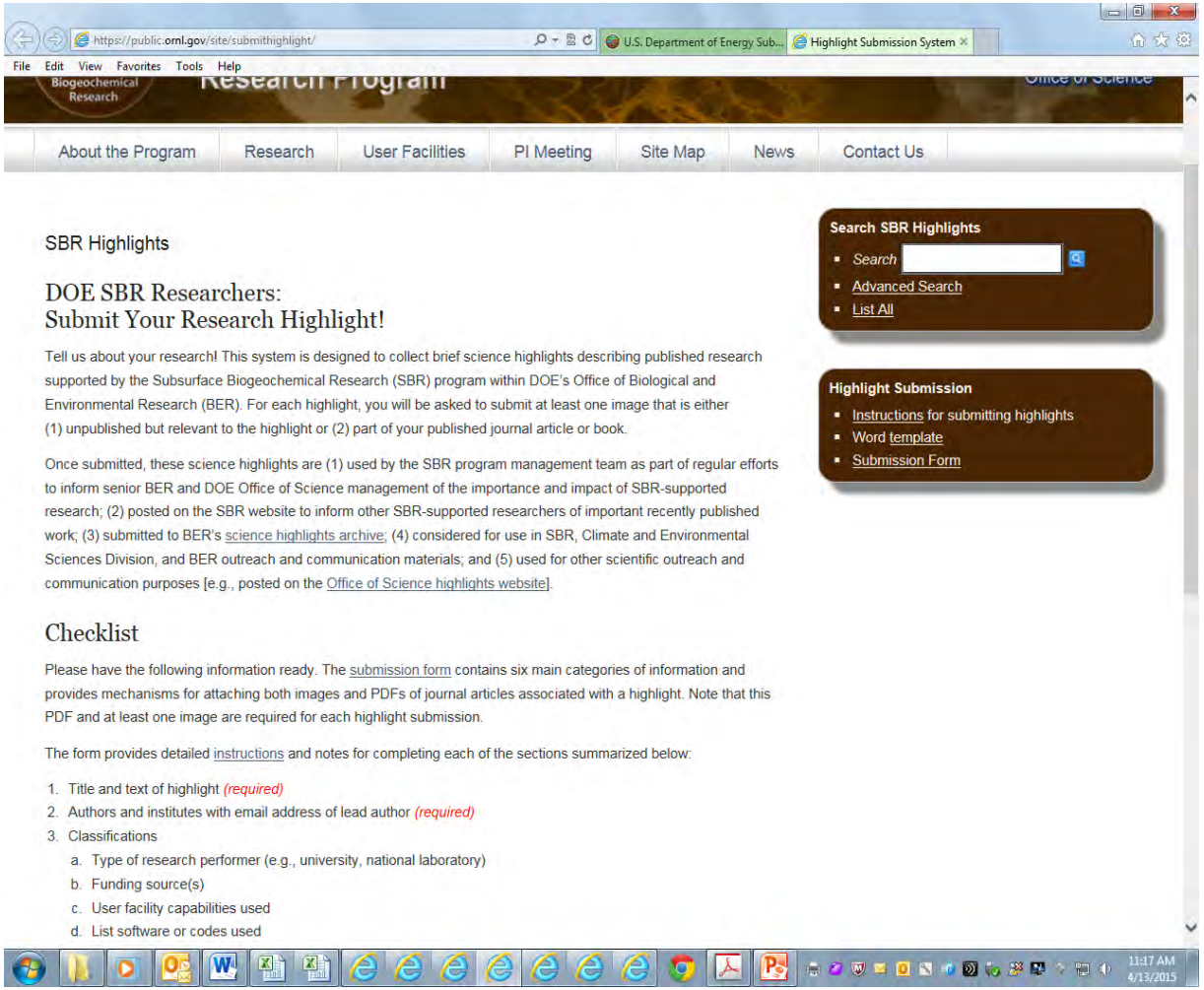
- 130 publications in 2013
- 110 publications in 2014
- 110 publications in 2015
- 32 publications (so far) in 2016

ASCE American Society of Civil Engineers

Walter L. Huber Civil Engineering Prize
M. Ye (U Central Fl) – 2015

Submit your Highlights!

Keep your SBR Program Manager and Fellow Scientists Informed

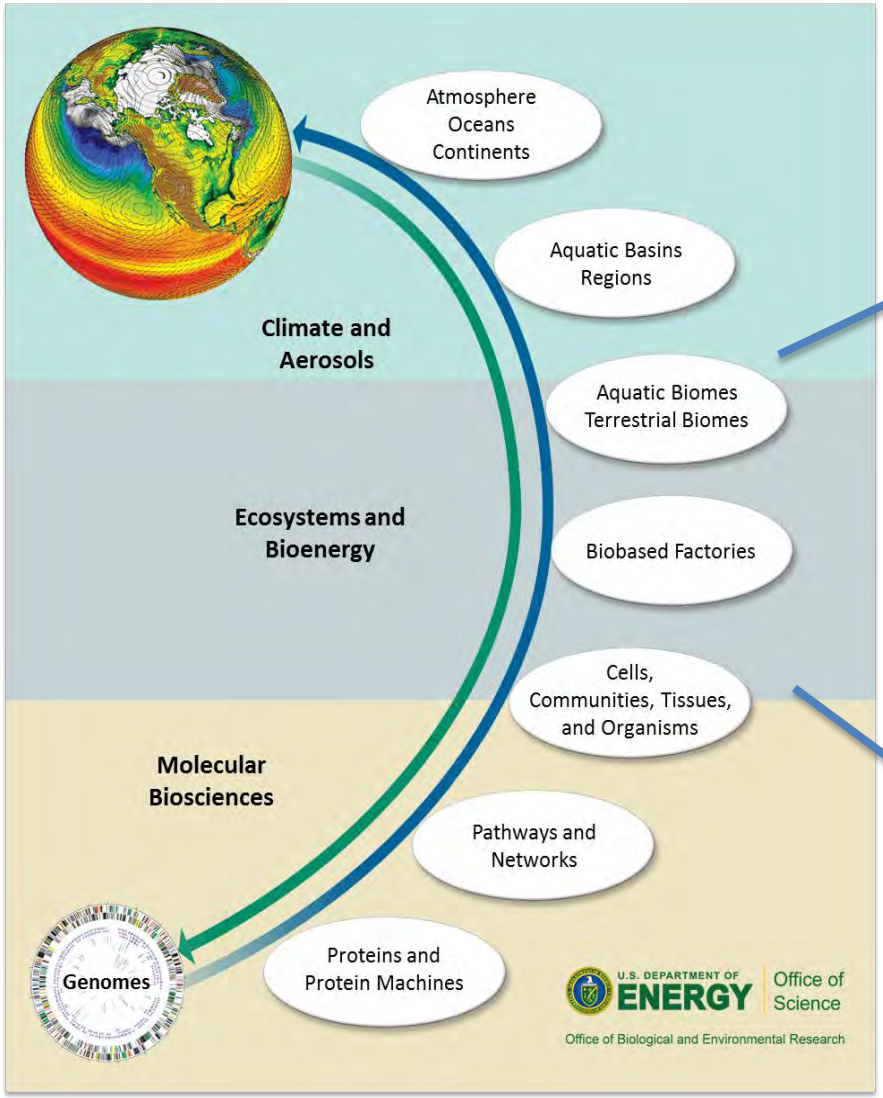


- *Inform the SBR program.*
- *Inform fellow scientists.*
- *Submit:*
  - *Paragraph*
  - *Graphic*
  - *pdf of your pub*

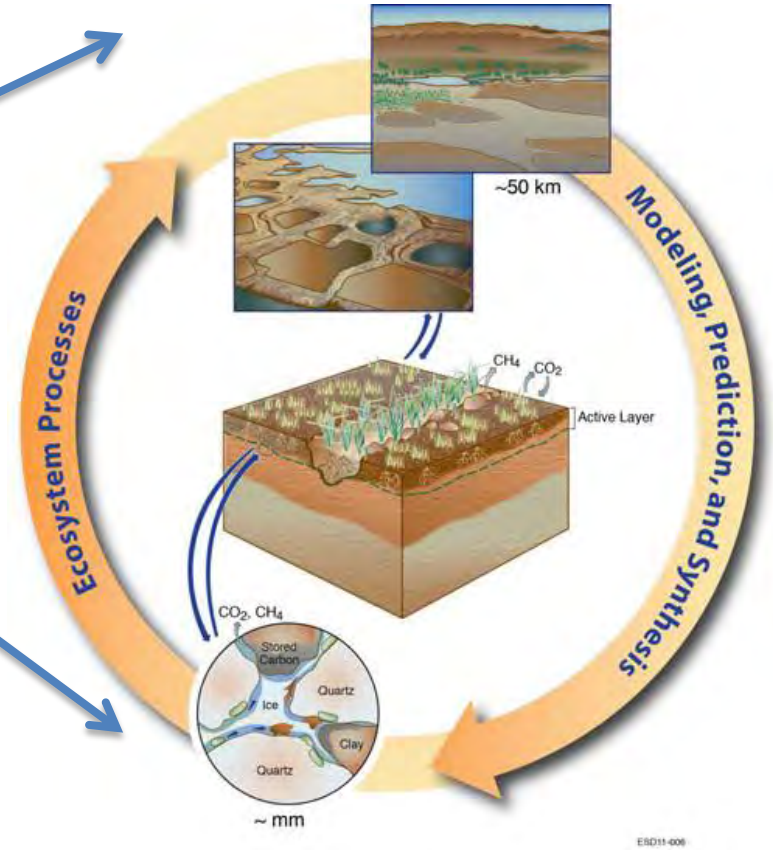
Web Page: https://public.ornl.gov/site/submithighlight/

Biological and Environmental Research

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



Environmental System Science:
Iterative approach used to advance predictive understanding of terrestrial environments ("MODEX")



ESS = TES + SBR Research Programs

Biological and Environmental Research

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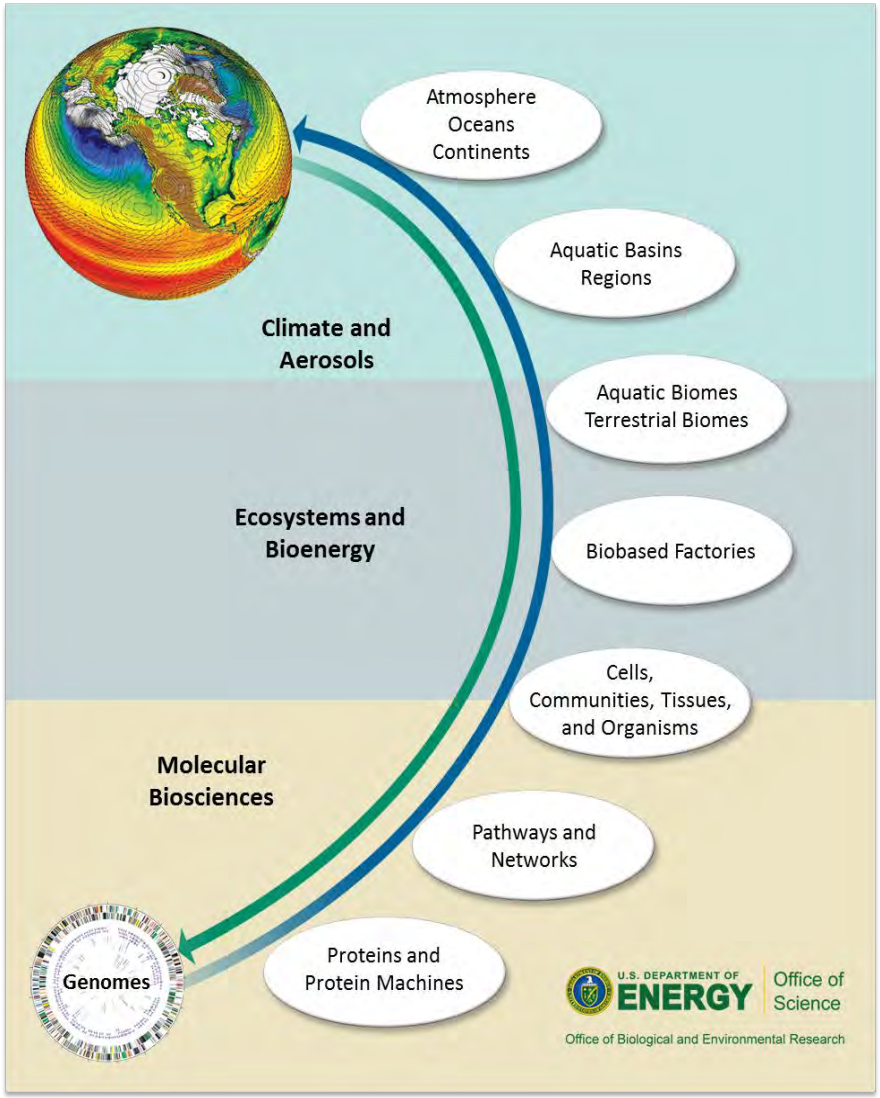
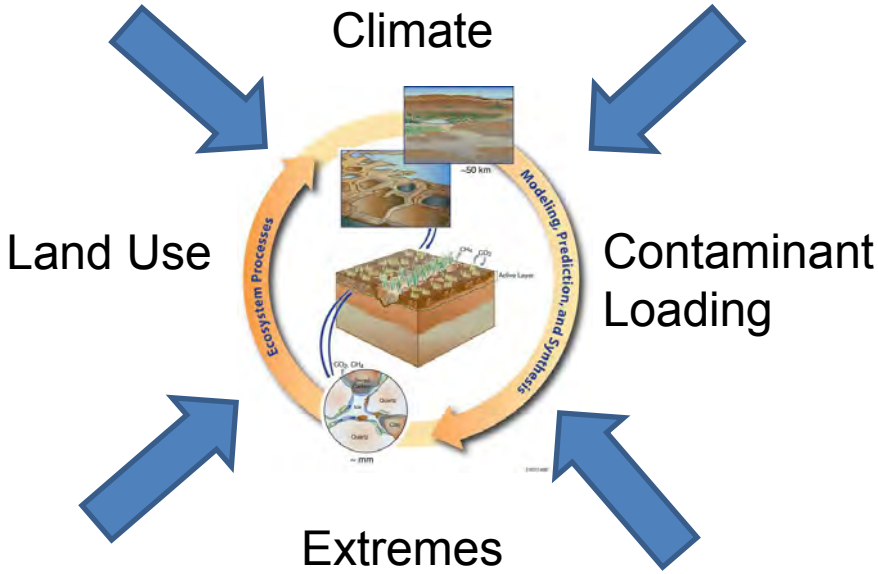


Watershed Function and Dynamics:

Mechanistic and Multiscale Understanding of Integrated System Response to Perturbations



DOE Energy and Environmental Mission

Inputs to Strategic Directions for SBR

BER Workshops and Reports

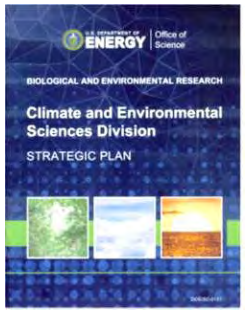
2008

BSSD
Carbon Cycle

2009

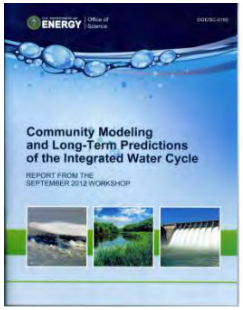
SBR
Complex Systems

2010



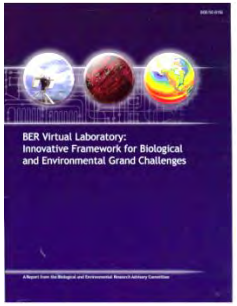
CESD
Strategic Plan

2012



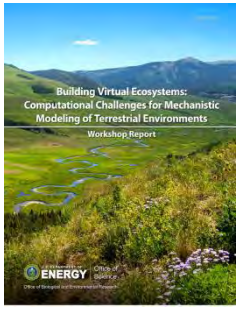
CESD
Integrated Water Cycle

2012



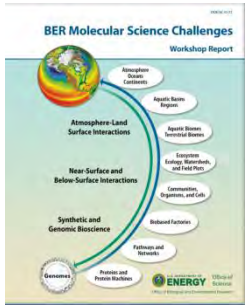
BERAC
Virtual Lab

2015



SBR
Building Virtual Ecosystems

2015



BER
Mol. Sci. Challenges

Broader Community: BES, ASCR, EM, LM, NSF, USGS, NOAA

2014

ASCR
Software \Productivity

2014

LBNL
Complex Soil Systems

2015

BES
Basic Research Needs for EM

2015

SOIL MODELING

Int. Conf.
Austin, TX

ISMC
Int. Soil Modeling Consortium

National CZO Program
CRITICAL ZONE OBSERVATORIES
funded by NSF
studying the zone where rock meets

CUAHSI
UNIVERSITIES ALLIED FOR WATER RESEARCH

CSDMS
COMMUNITY SURFACE DYNAMICS MODELING SYSTEM

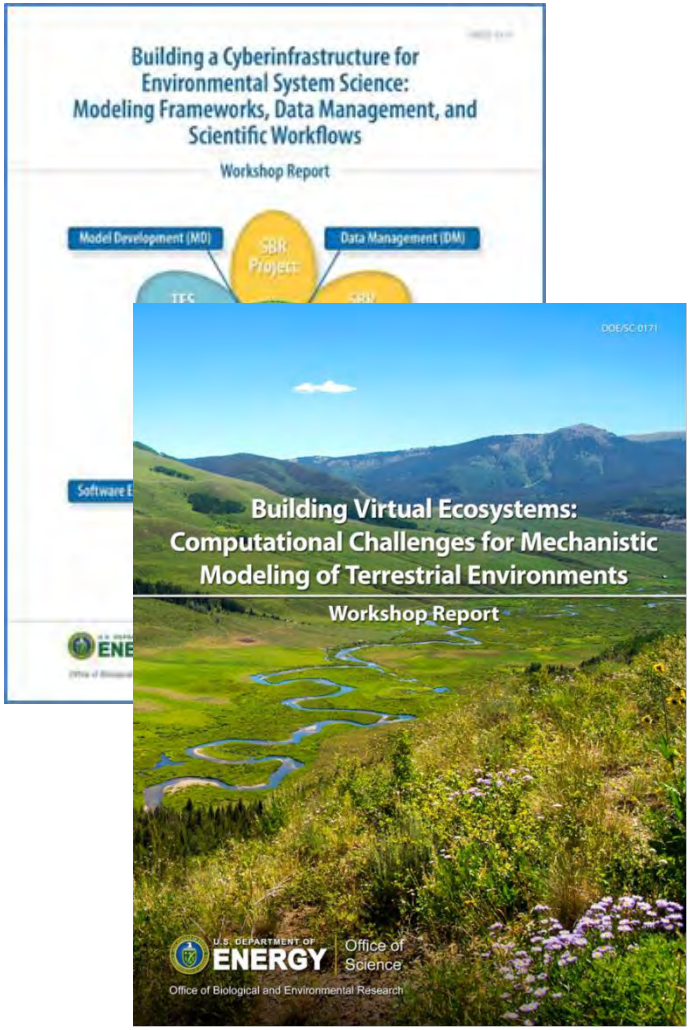
ISCMEM

NWC | NATIONAL WATER CENTER

SBR Goal: Mechanistic and Multiscale Understanding of Watershed Function & Dynamics – Genome Enabled BGC Models

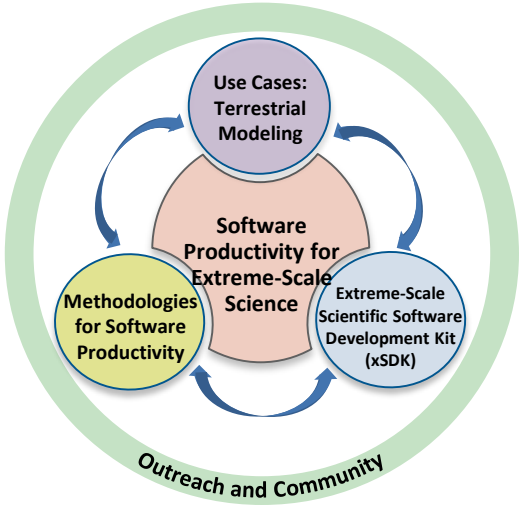
Building Community Infrastructure

Frameworks: Modular, Interoperable, Extensible; Data Management; Workflows



ASCR/BER: Software Productivity

IDEAS productivity

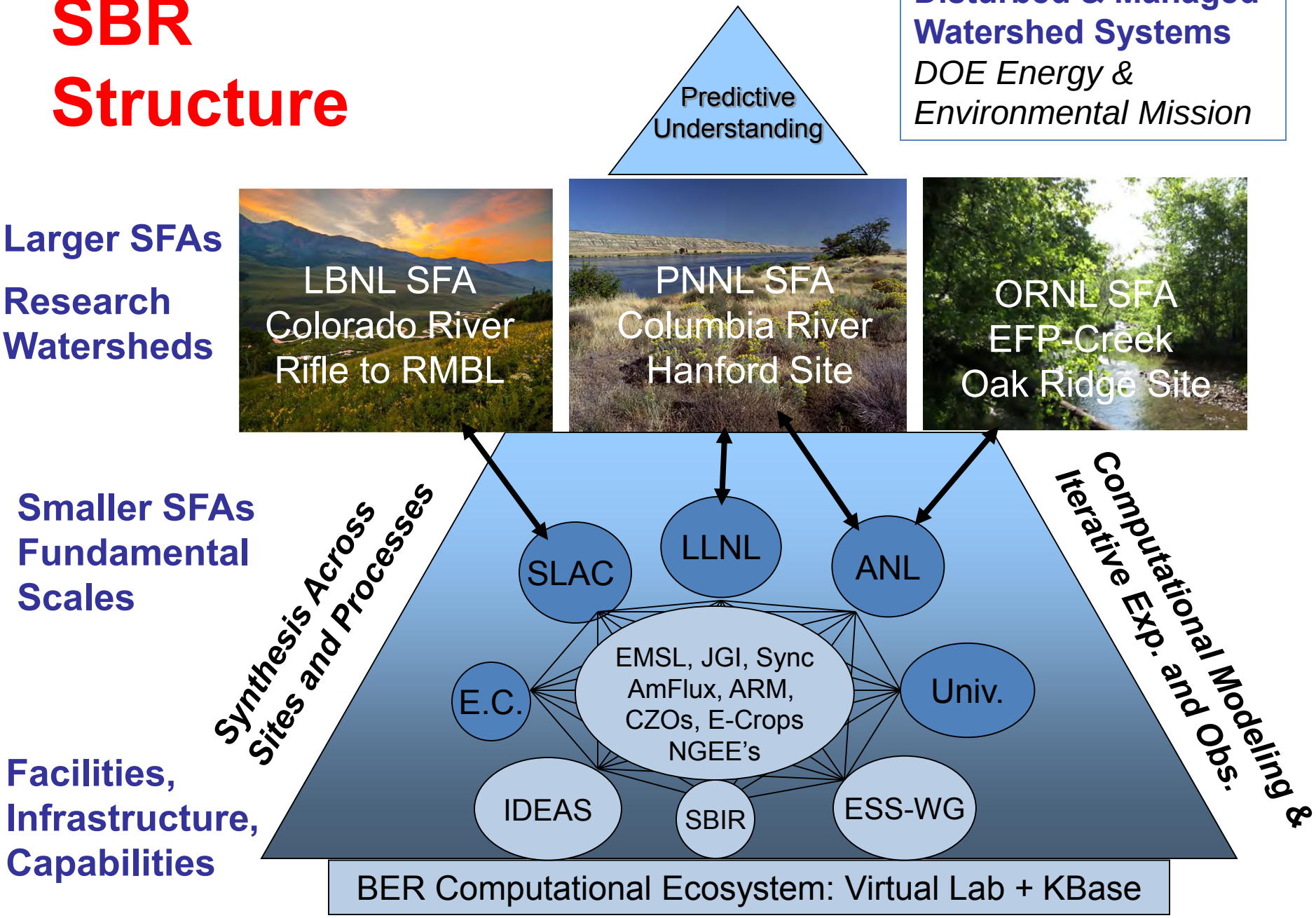


Disturbed & Managed Watersheds (SFAs-IDEAS)

LBNL SFA – U. Colorado R. Basin, Climate Impacts
PNNL SFA – Columbia R. Basin, Hanford Reach-U
ORNL SFA –East Fork Poplar Creek-TN, Hg Cycling
ANL SFA – Molecular BGC: U,Hg,Fe, S,C+microbes
SLAC SFA – Molecular BGC: U, C, Fe, S+microbes
LLNL SFA – Pu-Actinide BGC, Nevada Test Site
IDEAS UC1 – BGC Cycling, E. River Watershed, CO
IDEAS UC2 – Arctic Permafrost Dynamics
IDEAS UC3 – Integrated Hydrology, CONUS

SBR Structure

Disturbed & Managed Watershed Systems
DOE Energy & Environmental Mission



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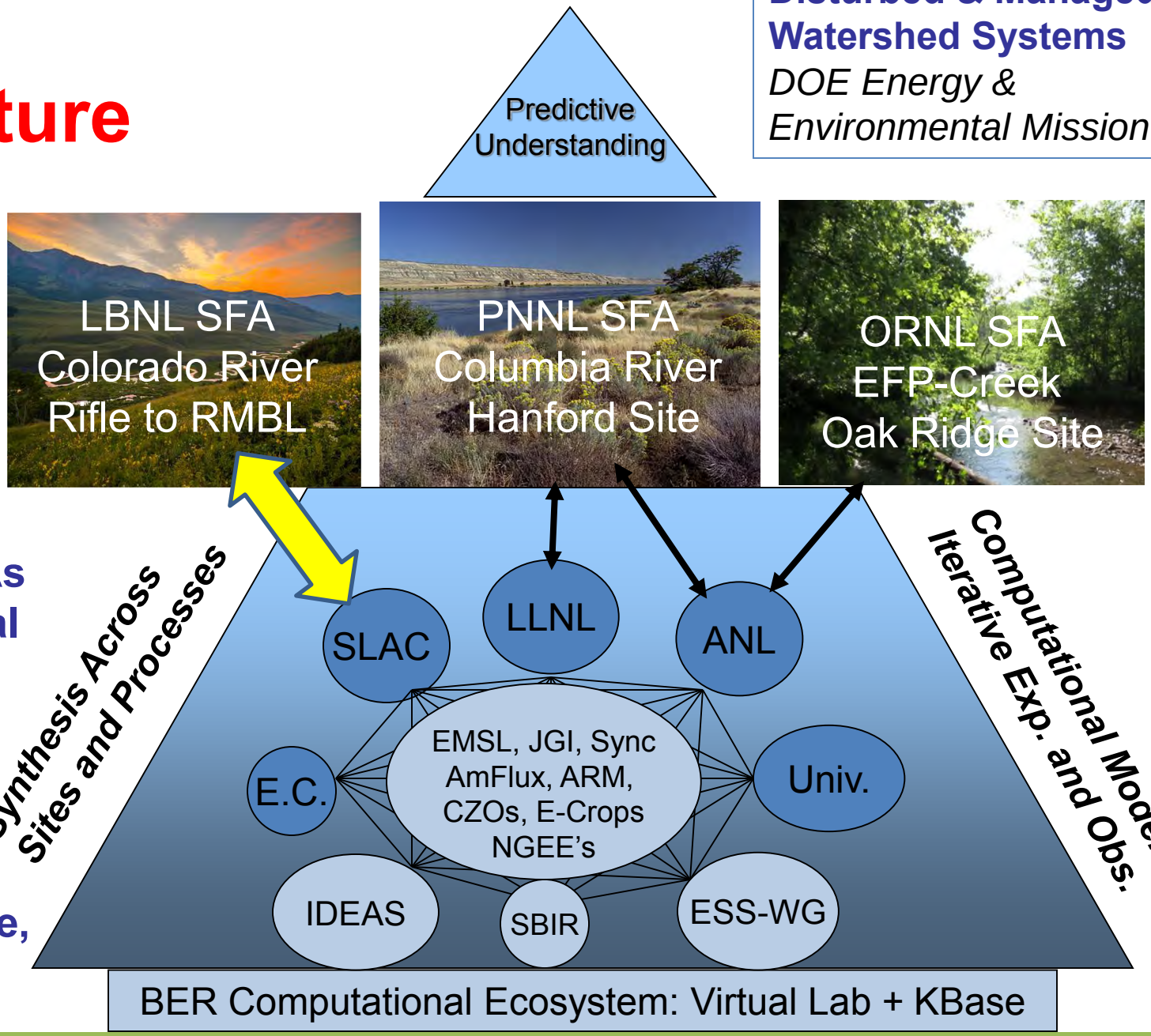
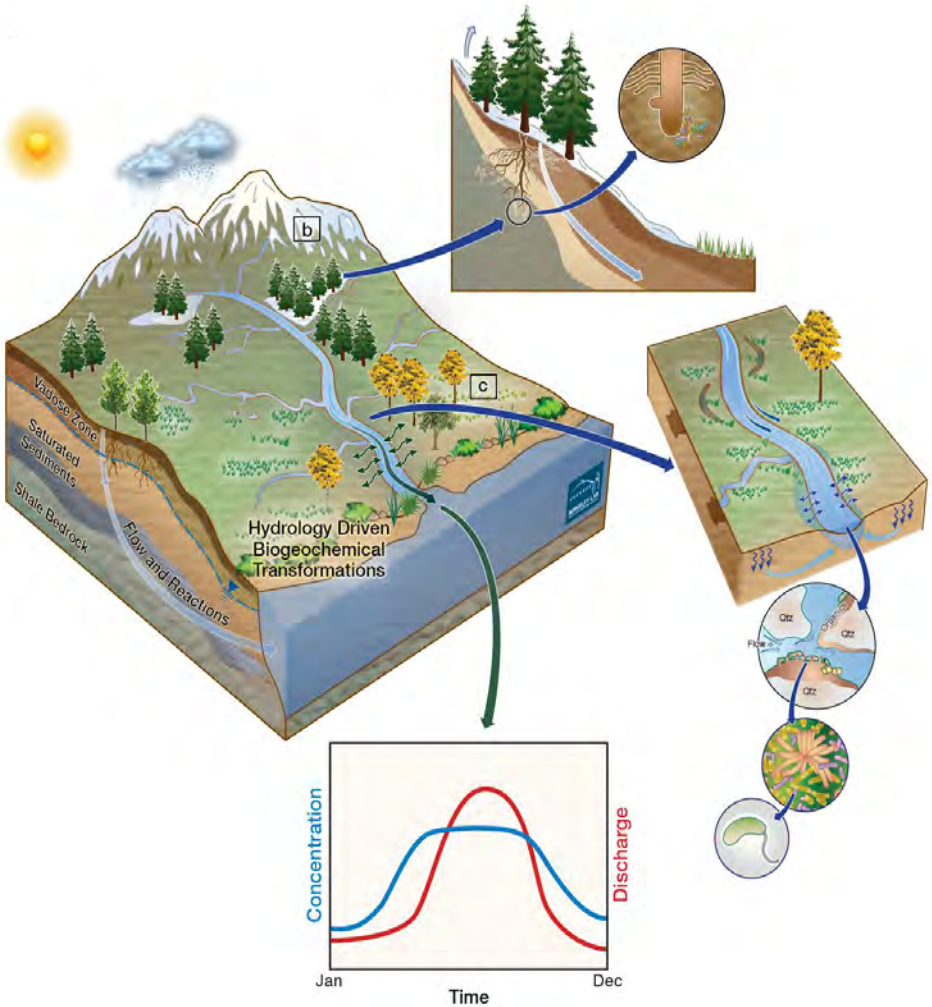


Berkeley Lab Watershed Function SFA:
Biogeochemical Dynamics from Genomes to Watershed Scales



http://watershed.lbl.gov/

Question: How do mountainous watersheds retain and release water, nutrients, carbon and metals?

- How will droughts, early snowmelt, and other perturbations influence mountainous watershed dynamics occurring from bedrock-to-canopy?
- How will these changes impact downstream water availability and biogeochemical cycling at episodic to decadal timescales?

Approach: System-of-Systems perspective & Scale-Adaptive Watershed Simulation Capability (SAWaSC)

- Adaptive mesh refinement to telescope into select subsystems, simulating fine scale processes only where and when they contribute to aggregated watershed response

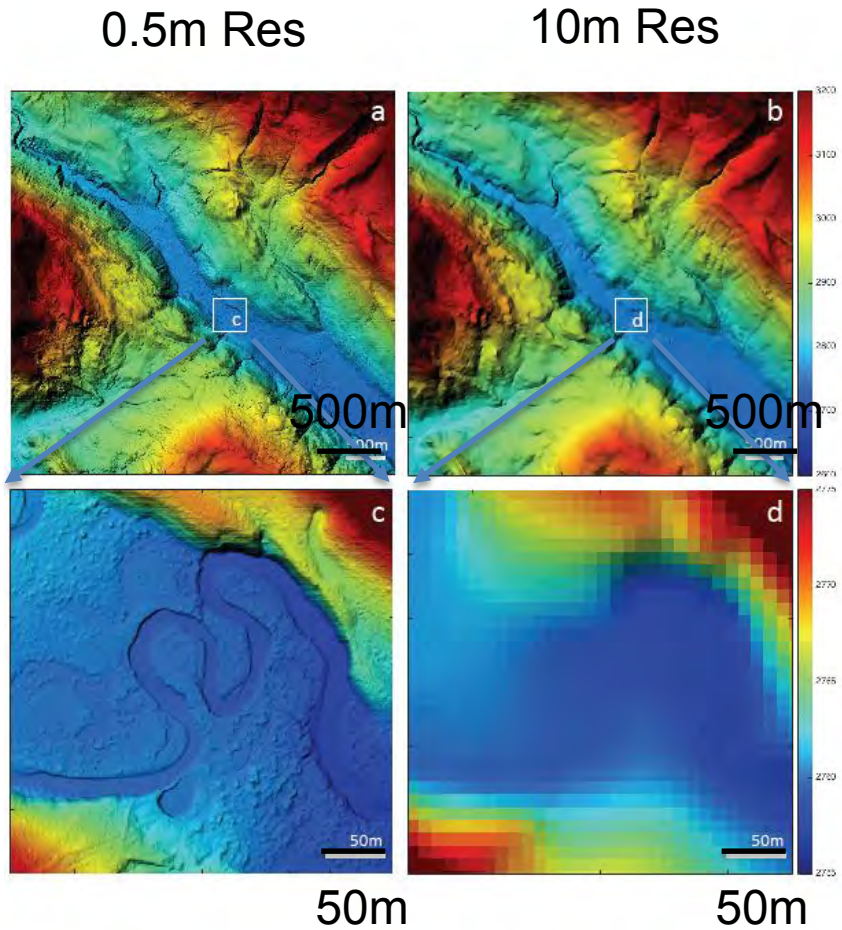
Testbed: Mountainous headwaters watershed, Upper CO River Basin

- Societally important, vulnerable to change

Mountainous Headwater Watersheds, CO
Perturbations to Water Availability

BERKELEY LAB

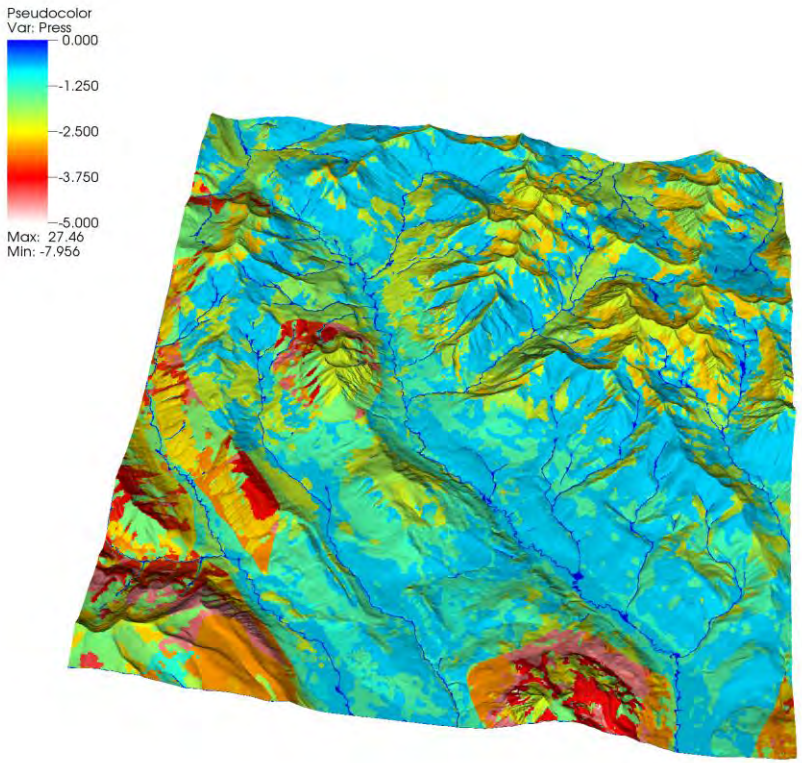
LBNL SFA East River Watershed Perturbations to Water Quality



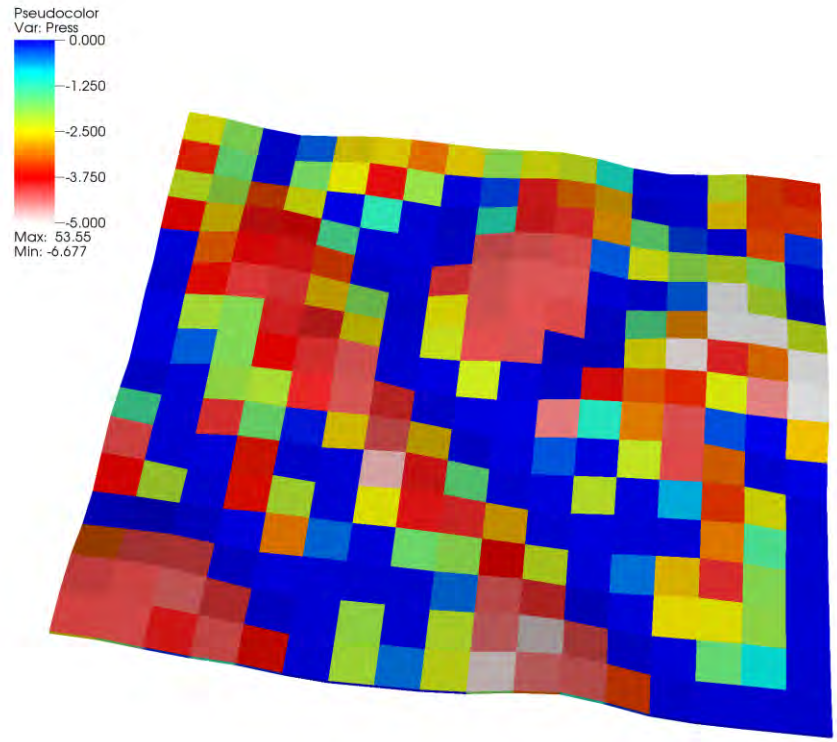
LBNL SFA East River Watershed

Modeling scale-dependent processes: $\overline{f(x)} \neq f(\bar{x})$

Question: What spatial and temporal scales are required to answer specific questions about water availability and water quality?



High resolution (10m)
ParFlow model [LBNL SFA]



Coarse resolution (1km)
ParFlow model [CONUS]

Courtesy: Reed Maxwell (CSM)

SLAC Science Focus Area

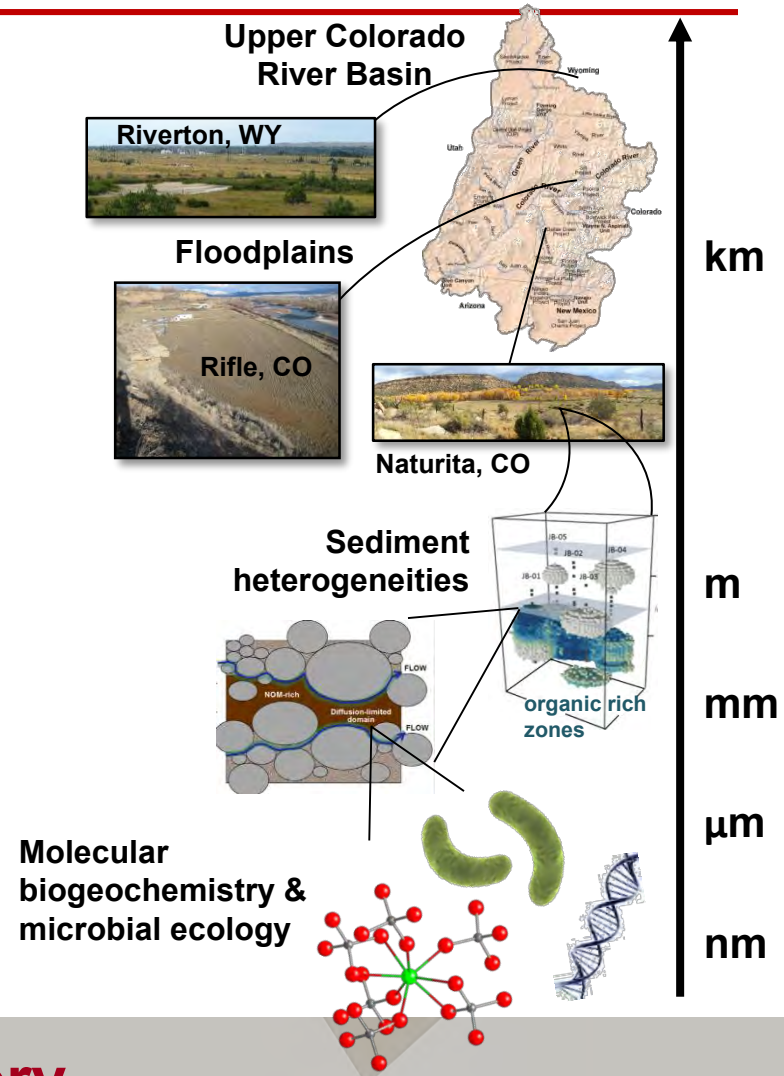
Coupled Cycling of Organic Matter, Uranium, and Biogeochemical Critical Elements in Subsurface Systems

SCIENCE QUESTIONS

- What are the molecular-to-meter scale controls over uranium mobility in organic-rich anaerobic sediments?
- Are anaerobic organic-rich sediments *regionally* important to uranium mobility and carbon and nutrient biogeochemistry?

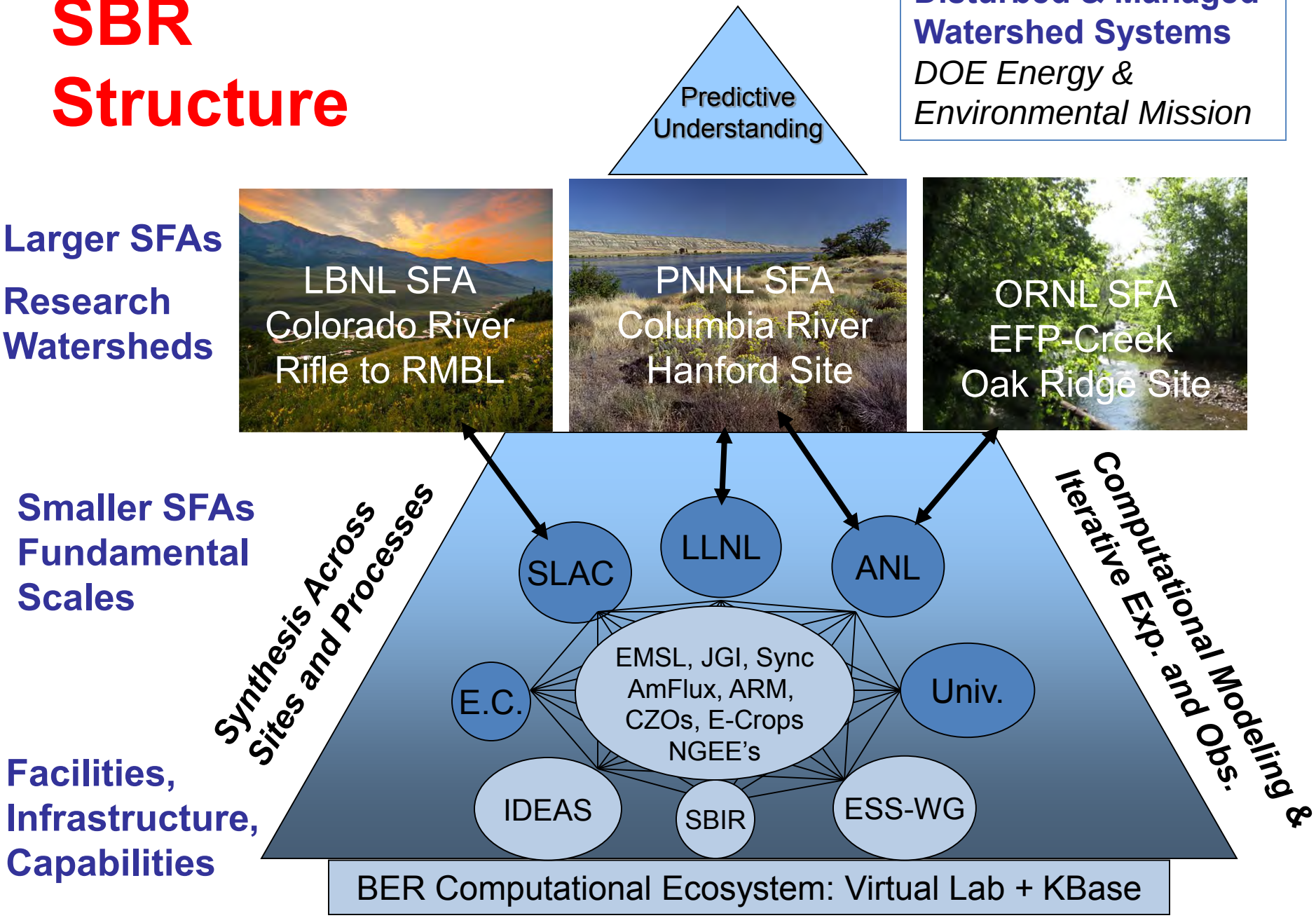
IMPACT

- Scale-aware biogeochemical process models for organic-uranium-nitrogen-iron-sulfur interactions
- Advances in our understanding of organic carbon reactivity in anaerobic sediments
- Biogeochemical model input parameters



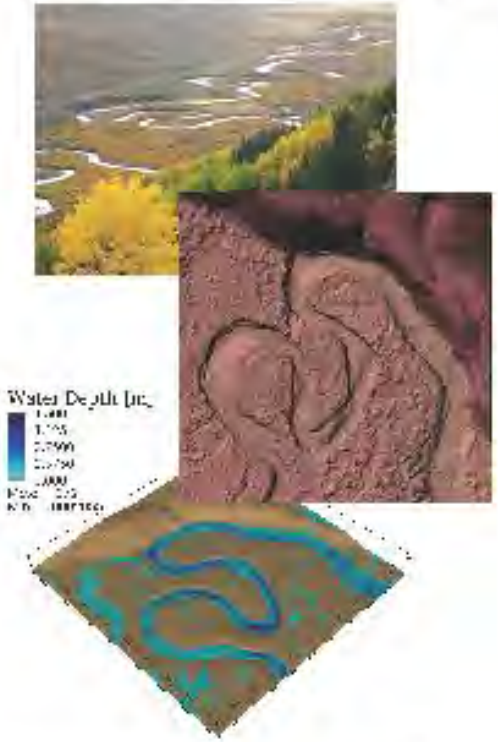
SBR Structure

Disturbed & Managed Watershed Systems
DOE Energy & Environmental Mission

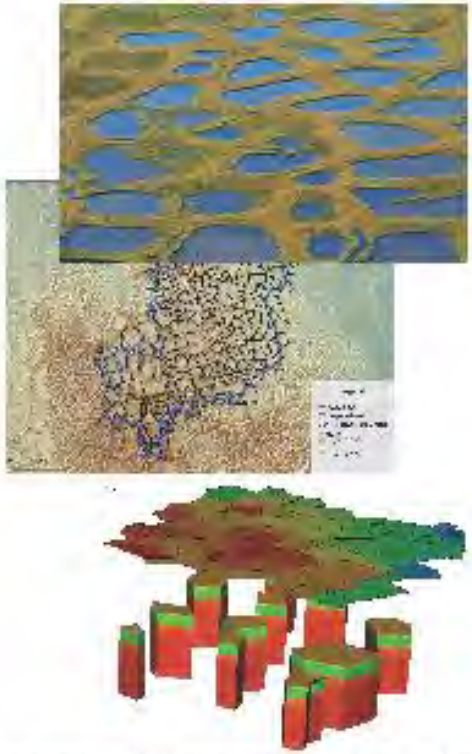


IDEAS productivity Interoperable Design of Extreme-scale Application Software (IDEAS)

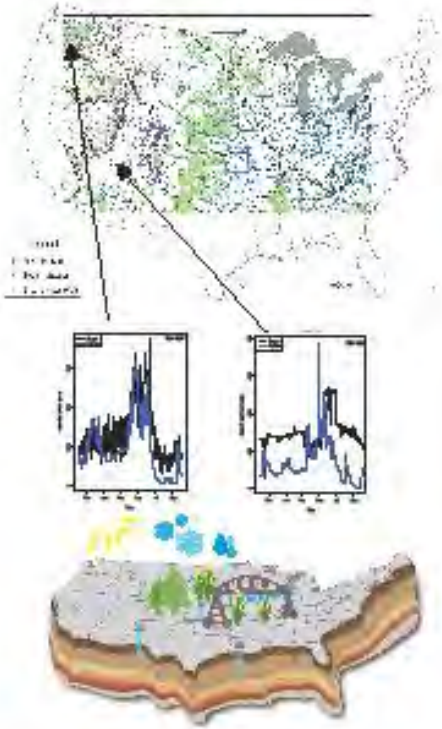
IDEAS multifaceted Use Cases use science drivers to motivate and explore software development productivity and interoperability to enhance scientific productivity.



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.

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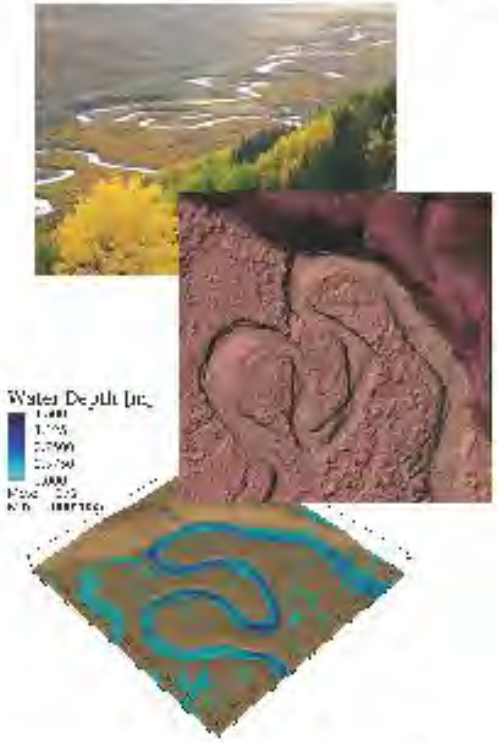

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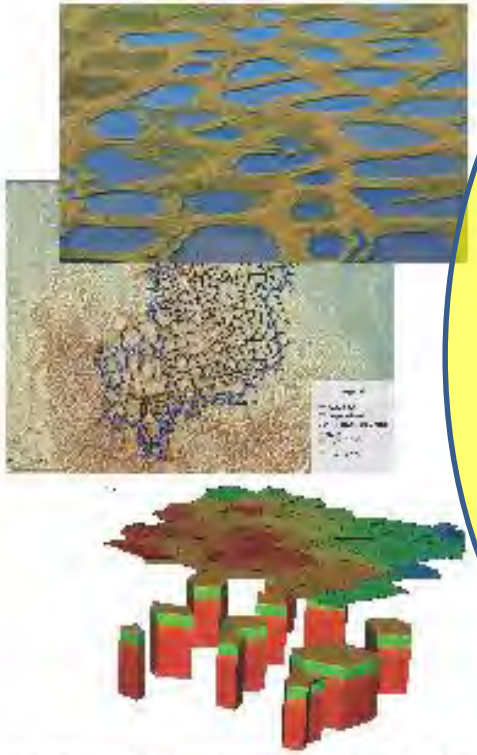

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CESD Coordination with National Water Model

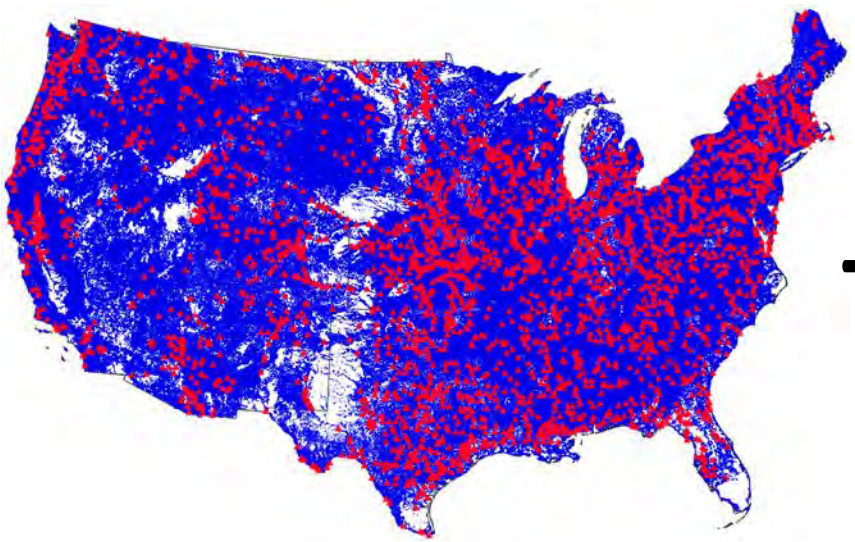
Integrated Water Prediction from Summits to Seas

Multiagency Effort led by NOAA (NCAR, USGS, USDA, EPA, NSF…)

=> SBR Focus on Disturbed & Managed Watershed Systems – Response to Perturbations
=> Enabling Mechanistic Assessments of Vulnerabilities, Impacts & Adaptation Strategies
=> Contribute to the Development of Hi-Fidelity National Testbeds (CONUS + AK)
=> Contribute to the Development of Seamless Weather-Climate Prediction Frameworks

NOAA: Surface Water Hydrology
WRF-Hydro Modeling Framework
7k => 2.7M river reaches ~1km res.

DOE: Hi-Res Integrated Hydrology – GW/SW
Modular and Extensible HPC Framework (+RTM)
Currently ~1km res. => Variable Res; AMR



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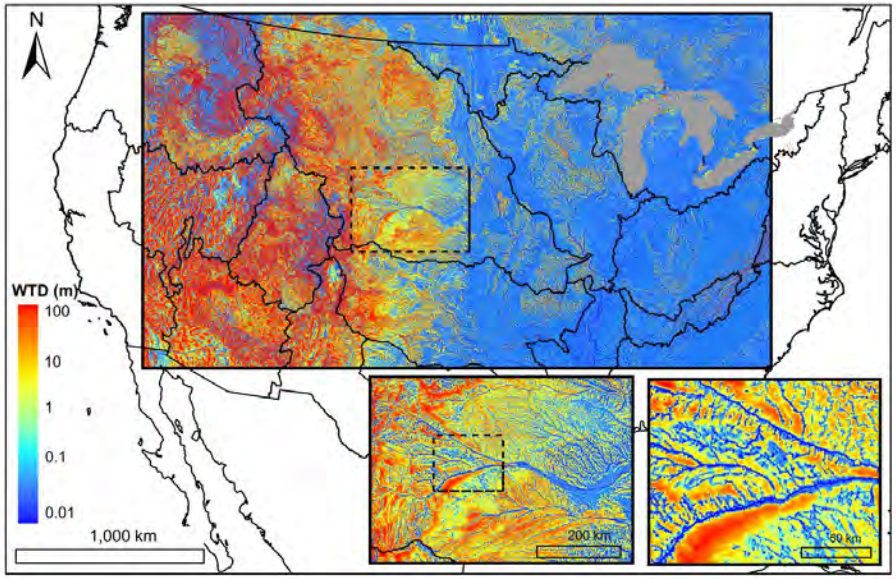
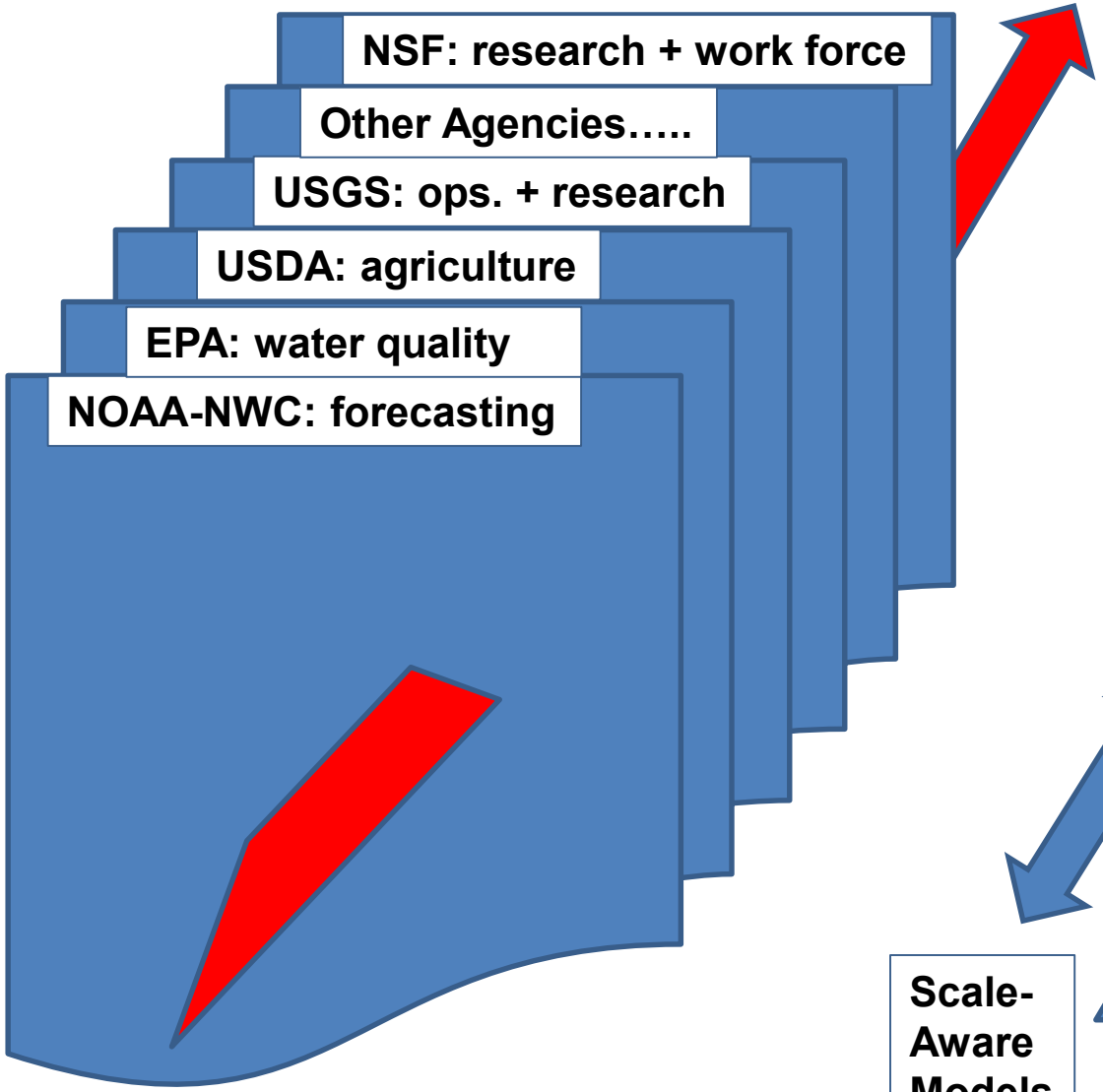


NWM Simulations: https://www.youtube.com/watch?v=lbA2KoYSEsg

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"

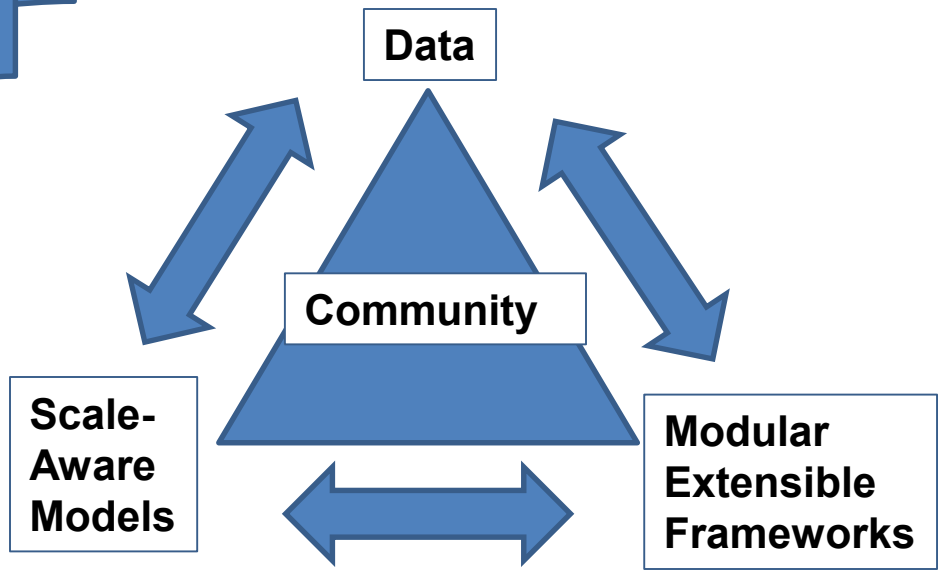
But incomplete….

>Local test beds with specific focus

>Missing system components

>Need data from external sources

Research + Operations = Win-Win



Solicitations

- ESS University Solicitation
  - FY15: SBR made 5 awards
  - FY16: Solicitation – SBR anticipates making 5 to 10 awards
    - SBR component CONUS focus and complimentary to SFA's ($600k/3yrs)
    - Lab contribution limited to 10% of total award
  - FY 17: SBR planning for a similar FOA
- Small Business Innovative Research (SBIR)
  - Technologies for Subsurface Characterization and Monitoring
- BER Early Career Solicitation: Lab and University Awards
  - Previous SBR Awardees: Matt Marshall (PNNL), Helen Hsu-Kim (Duke), Ming Ye (FSU); Joel Rowland (LANL)
  - FY 15: Land-Atmosphere Interactions – Jonathan Raff (Indiana U.)
  - FY 16: Tropical Forests and IA-ESM Modeling– TBD

- ARPA-E: ROOTS FOA (concept papers due 5/26/16)
  - Rhizosphere Observations Optimizing Terrestrial Sequestration

Predictive Understanding of

Watershed Function and Dynamics

Genomes to Watershed, Disturbed and Managed

Near Term Step to Advance BER Goals: National Water Model

Resources:

SFAs in critical testbeds, deep hydro-biogeochemical expertise, modern computational & data tools

..to enable new Scientific Insights

- How do subsystem processes aggregate to yield a cumulative watershed response?
- Which, where and when do fine-scale biogeochemical processes significantly influence watershed behavior?
- How do extreme events propagate along lateral gradients?

..at scales and with accuracy to inform BER-relevant IAV

- Water-energy
- Sustainable bioenergy
- Watershed-basin responses to extreme events – droughts, floods, fires
- Contaminant transport

..to advance Broader BER Goals

- Next generation watershed science and scale-adaptive models to underpin solutions to Nation's environmental challenges.
- Bridge ESS
- Inform ACME development

Predictive Understanding of

Watershed Function and Dynamics

Genomes to Watershed, Disturbed and Managed

Longer Term: => Seamless Weather-Climate Terrestrial Prediction Framework

Resources:
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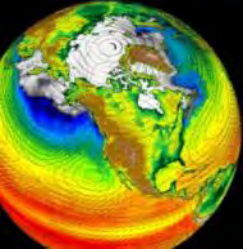
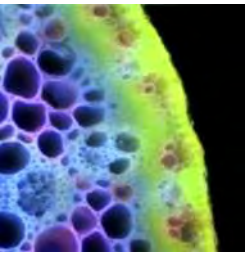
Leveraging Community Resources

- *Monday:* CESD-ESS Cyberinfrastructure Working Group
  - Briefing from David Moulton, Acting Chair of Executive Committee
- *Tuesday:* Lunch with ASCR Program Managers
  - Lucy Nowell, Carolyn Lauzon, Thomas Ndousse-Fetter
- *Tuesday Evening*: Community Modeling of Soil Systems
  - Michael Young, Co-Chair of Austin International Conference
  - Panelists: Chen, Faybishenko, Maher, Painter, Papchepsky
- *Wednesday PM - Final Plenary:*

Water-Energy-Land Nexus: Understanding and Managing System Complexity and Dynamics

- Hoyt Battey (DOE-EERE), Edward Clark (NOAA-NWC), Donald Cline (USGS), Thomas Torgersen (NSF), Bob Vallario (DOE-BER)





Questions?

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david.lesmes@science.doe.gov

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

Roland Hirsch, BSSD
roland.hirsch@science.doe.gov

SBR Website: doesbr.org

Building a Cyberinfrastructure for Environmental System Science: Modeling Frameworks, Data Management, and Scientific Workflows

Workshop: April 30 – May 1, 2015; Potomac, MD
DOE Organizers: David Lesmes and Jay Hnilo
Workshop Chair: David Moulton, LANL (9 people on Organizing Committee)
Participants: 36 participants from 8 National Laboratories (SBR, TES, ASCR)
Goal: Inform Development of ESS Working Groups for Model-Data Integration
Report: http://doesbr.org/ESS-WorkingGroups/.

Next Steps:

Establish ESS-WG Steering Committee

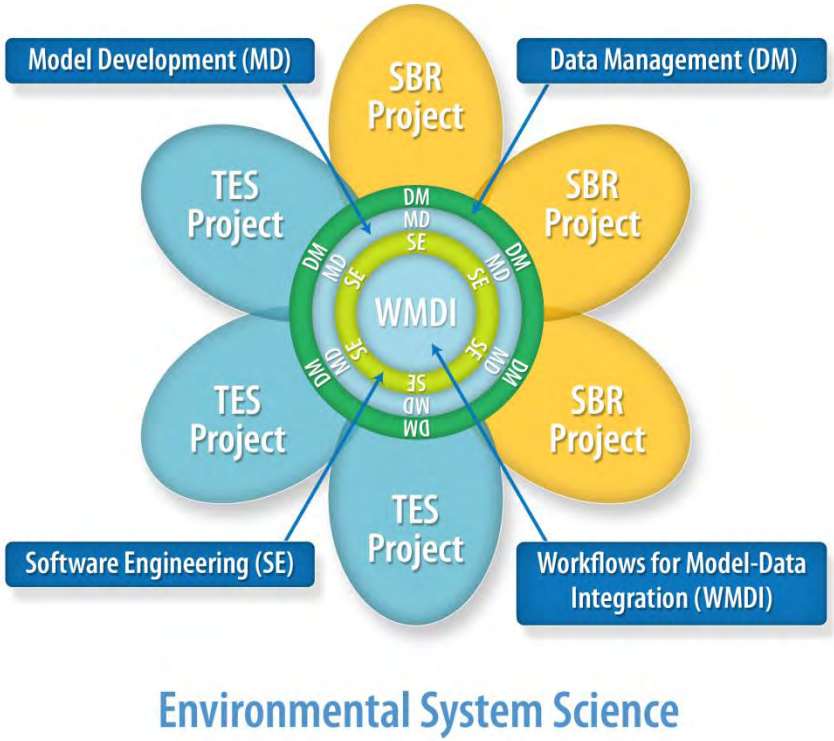
- 4 TES Reps (NGA, NGT, SPRUCE, AmFlux)
- 4 SBR Reps (SFAs: LBNL, PNNL, ORNL; IDEAS)
- ~2 External Reps

Establish 2 to 4 ESS Working Groups

- **Data Management**
- **Model-Data Integration**
- **Software Engineering and Interoperability**
- Community Governance
- *WG dissolved when task complete!*

Reporting on Working Group Task Status

- Quarterly reporting to S.C. (PMs) and E.C. (PIs)
- Annual reporting at ESS PI Meeting



EXTRA SLIDES

Richard Dean "Dick" Dayvault
May 6, 1948 - August 29, 2015

Join us to honor and remember an amazing man and, in lieu of flowers, please bring a favorite "rock" to donate to the Dayvault Memorial Rock Garden.

Interoperable Design of Extreme-scale Application Software (IDEAS)

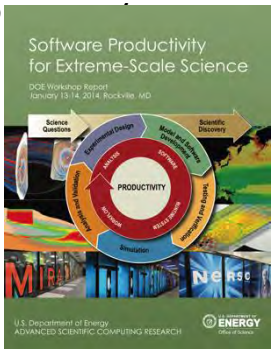
Motivation

Enable ***increased scientific productivity,*** realizing the potential of extreme- scale computing, through ***a new interdisciplinary and agile approach to the scientific software***

Objectives

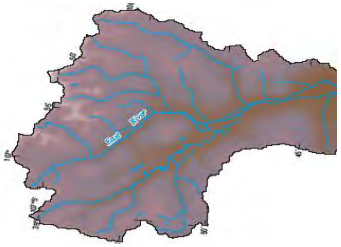
Address confluence of trends in hardware and increasing demands for predictive multiscale, multiphysics simulations.

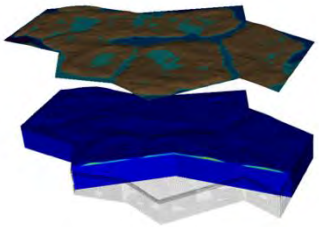
Respond to trend of continuous refactoring with efficient agile software engineering methodologies and improved software design.



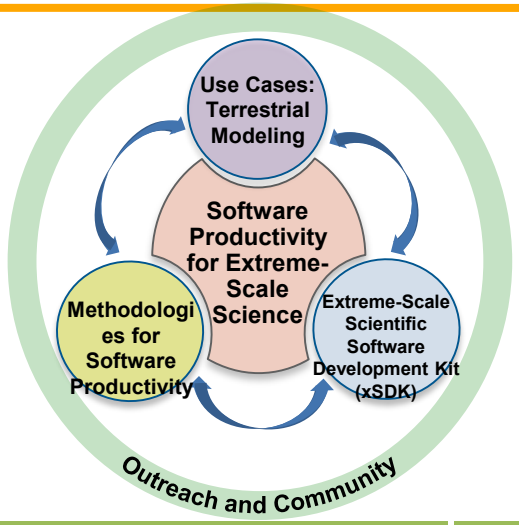
Impact on Applications & Programs

Terrestrial ecosystem ***use cases tie IDEAS to modeling and simulation goals*** in two Science Focus Area (SFA) programs and both Next Generation Ecosystem Experiment (NGEE) programs in DOE Biologic and Environmental Research (BER).





Approach



ASCR/BER partnership ensures delivery of both crosscutting methodologies and metrics with impact on real application and programs.

Interdisciplinary multi-lab team (ANL, LANL, LBNL, LLNL, ORNL, PNNL, SNL)

ASCR Co-Leads: Mike Heroux (SNL) and Lois Curfman McInnes (ANL)

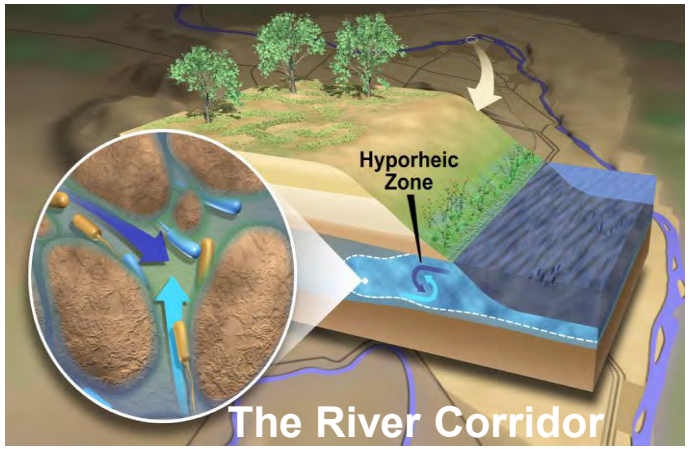
BER Lead: David Moulton (LANL)

Topic Leads: David Bernholdt (ORNL) and Hans Johansen (LBNL)

Integration and synergistic advances in three communities deliver scientific productivity; outreach establishes a new holistic perspective for the broader scientific community.

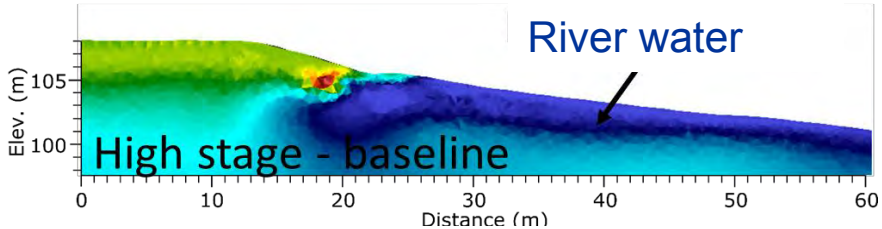
http://ideas-productivity.org/

PNNL SBR-SFA: Hydrobiogeochemical Process Dynamics in the Groundwater-Surface Water Interaction Zone



Goal: Understand, model, and predict coupled hydrologic and biogeochemical processes controlling carbon, nutrient, and contaminant behaviors in the groundwater – surface water interaction zone of a managed, river corridor system

Geophysical monitoring of river intrusion

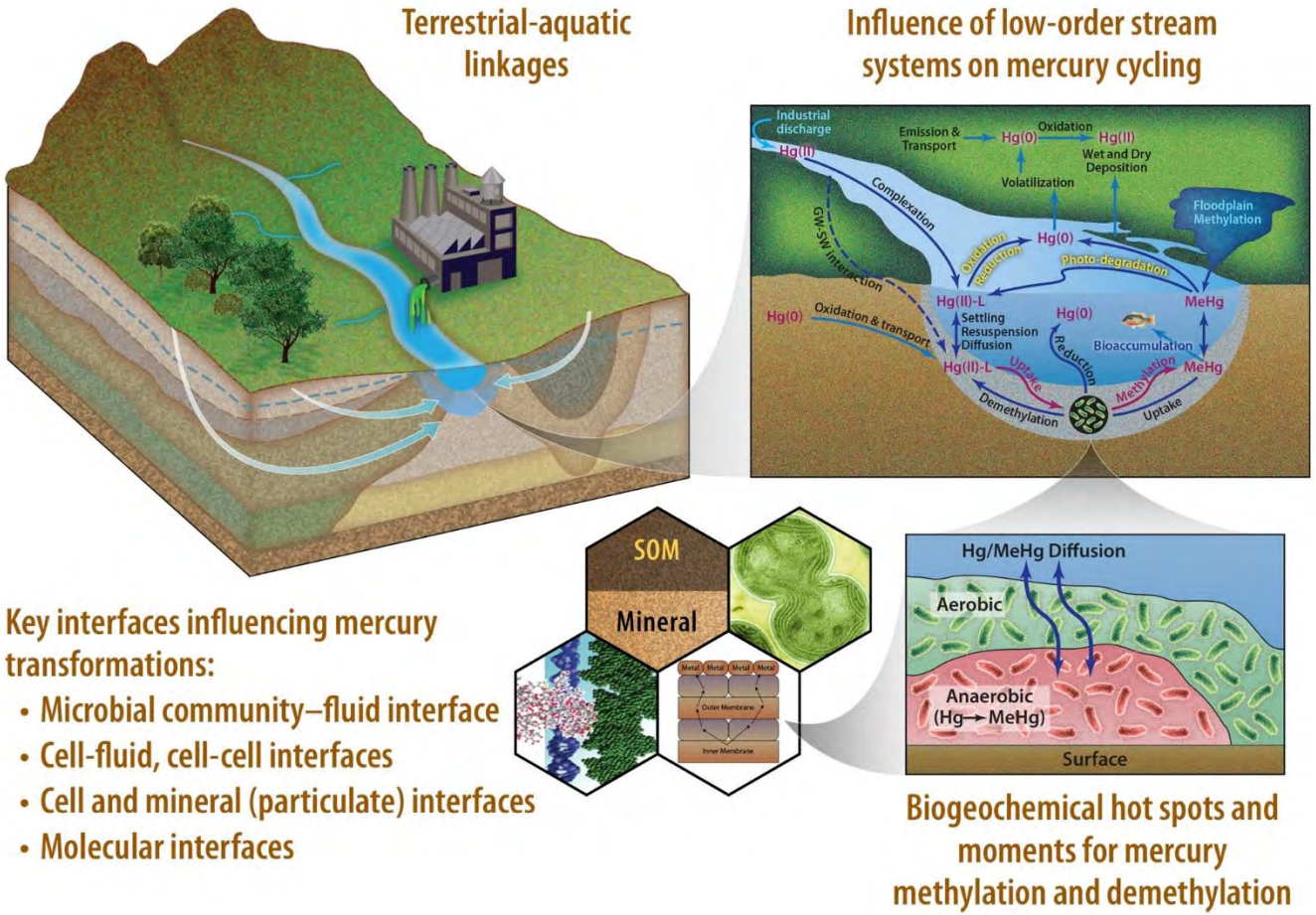


Sampling gas and water from the interaction zone

Research Activities

- Observing dynamic groundwater-surface water mixing impacts through robust time series monitoring.
- Field and laboratory experiments of coupled hydrologic and microbiologic processes and mechanisms.
- Organic carbon dynamics, speciation, and functional enzyme concentrations.
- Multi-scale ecologic , biogeochemical, and hydrologic research and models.
- Coupled land surface – subsurface – riverine models at the reach scale
  Water residence time as a key variable.

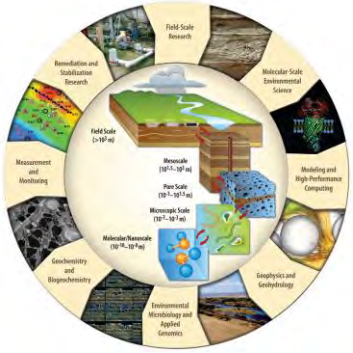
ORNL Scientific Focus Area
Biogeochemical Transformation at Critical Interfaces



Science Challenge: *Determine the coupled hydrobiogeochemical processes that control mercury fate and transformation in low-order freshwater stream systems.*

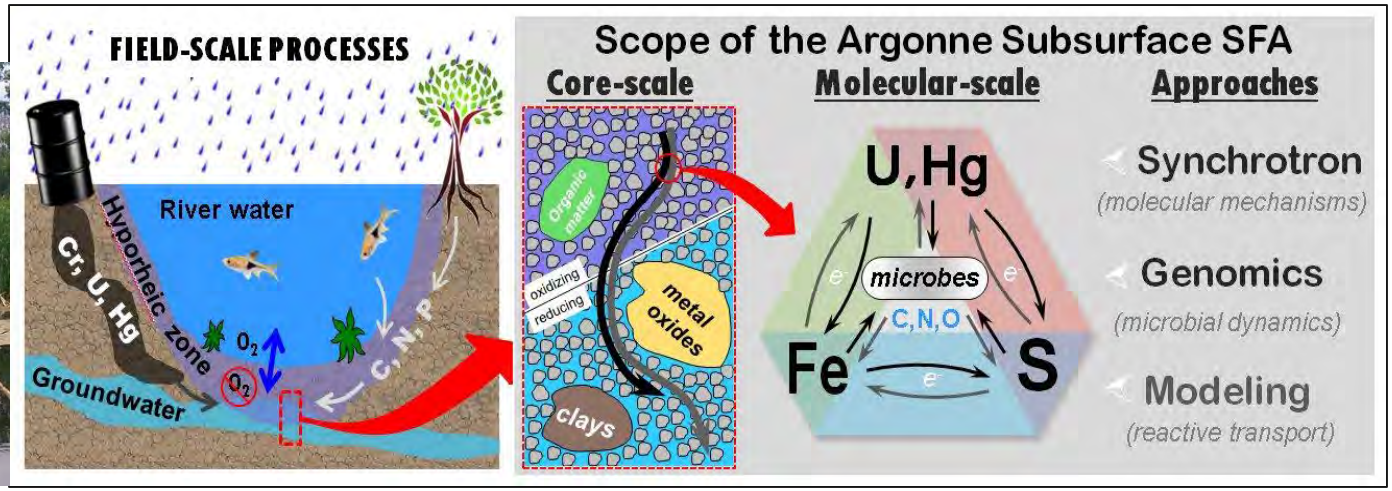
Science Goal: *Process-rich predictive capability that integrates field, laboratory, and modeling studies of mercury fate and transformation dynamics across broad spatiotemporal scales in low-order streams.*

Argonne SBR SFA: Fe and S Biogeochemistry in Redox Dynamic Environments



KBase
PREDICTIVE BIOLOGY

Understanding coupled biotic-abiotic molecular to core-scale transformations of Fe and S within redox-dynamic environments and the effects of Fe and S biogeochemistry on the transformation and mobility of major/minor elements and contaminants.

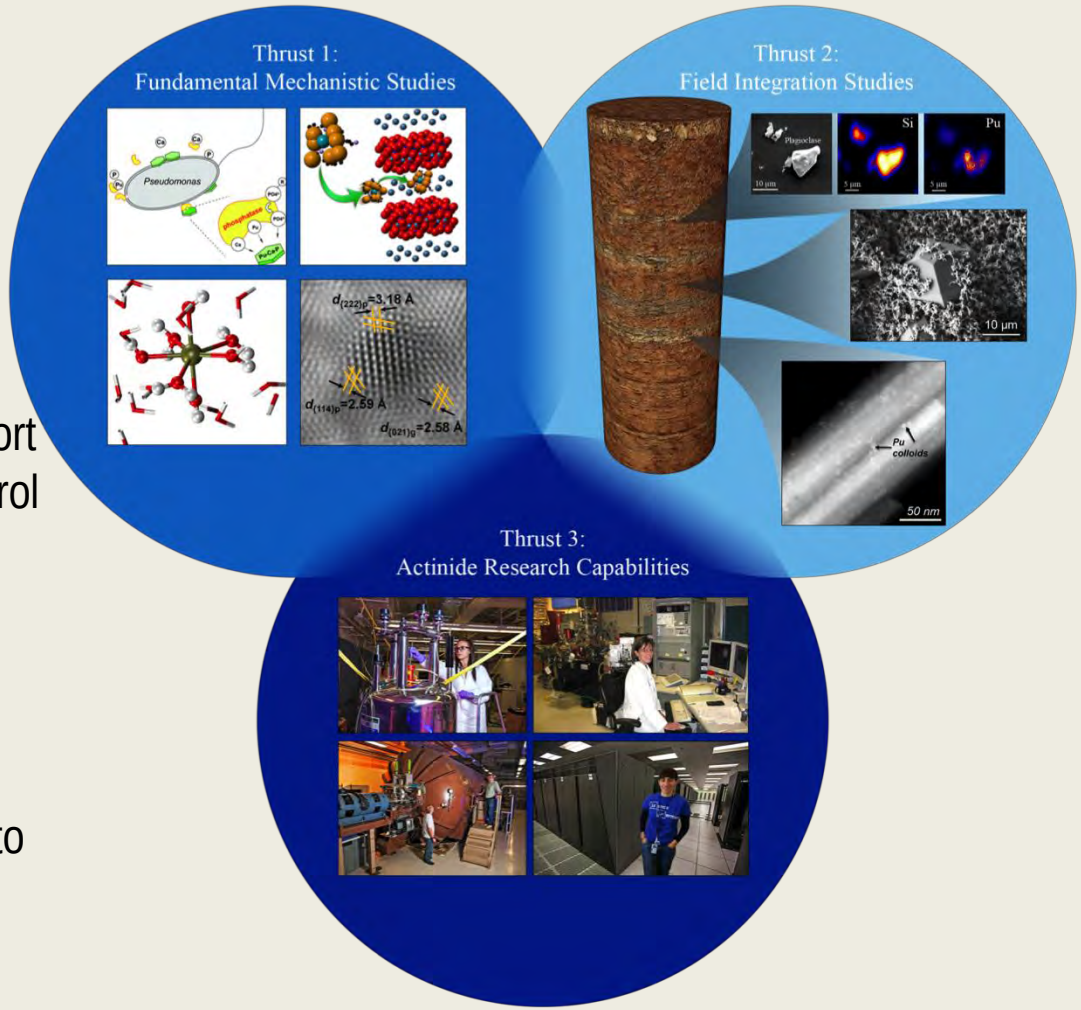


LLNL SFA: Subsurface Biogeochemistry of Actinides

- Justification: Advance our understanding of actinide behavior to enable actinide remediation, long-term stewardship, & safe storage

- Mission: Identify the dominant biogeochemical processes and mechanisms controlling actinide transport (Pu and Np) to reliably predict and control cycling and mobility of actinides in the subsurface

- Approach: Integrate molecular-scale mechanistic investigations and field studies. Advance research capabilities to achieve our scientific goals.

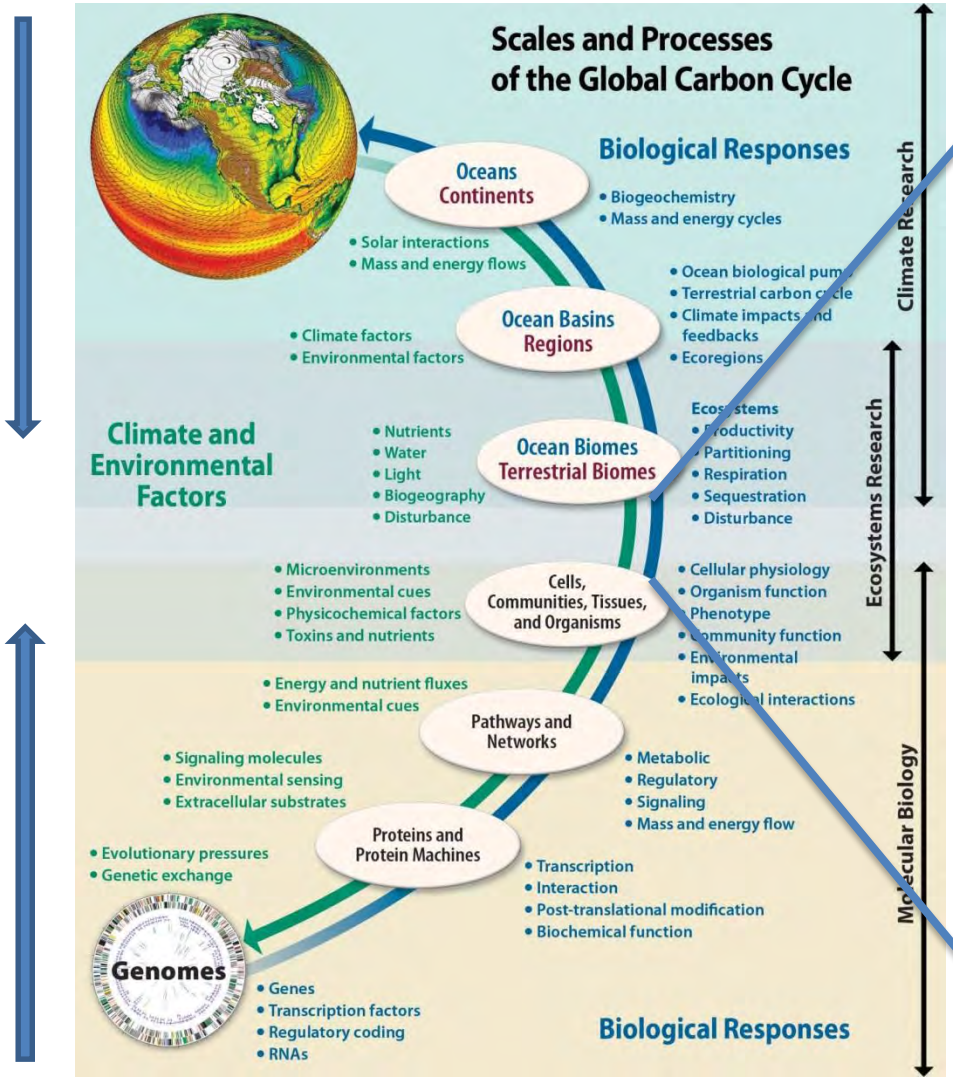


Path Forward

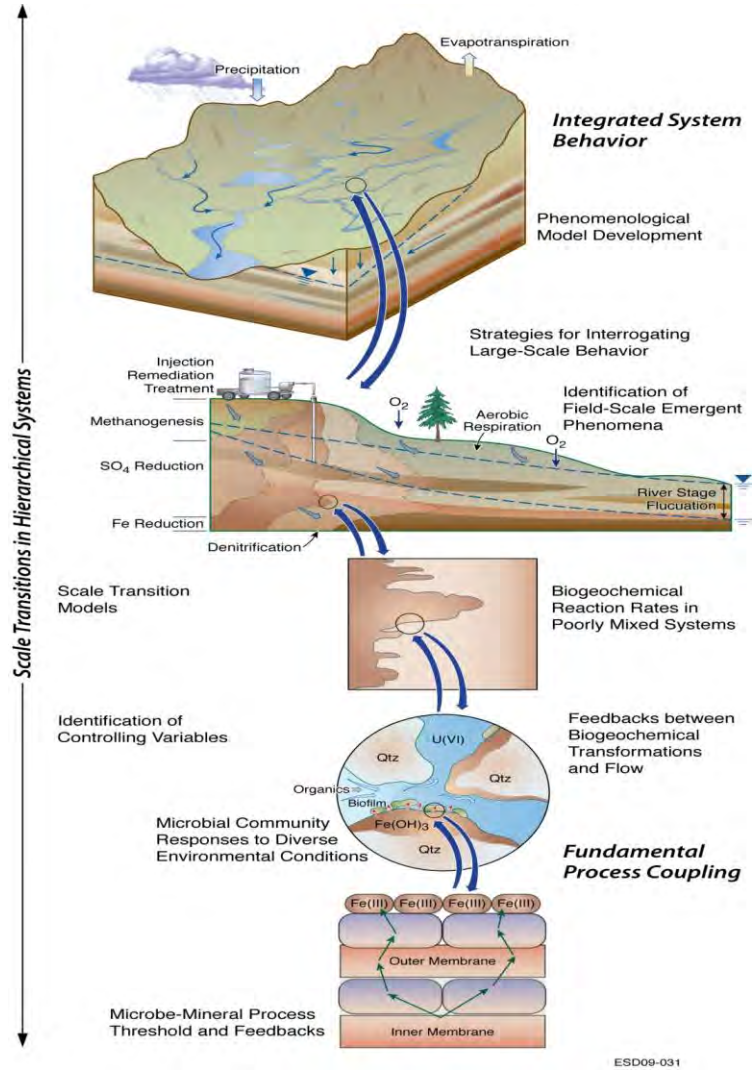
- Leverage IDEAS Use Cases and SFAs to Contribute to National Water Modeling Framework
  - Work with NOAA and interagency partners to enhance community approach to mechanistic modeling of terrestrial systems
- Focus on Disturbed and Managed Systems within CONUS
  - Use Cases driven by DOE mission relevance, societal importance and elucidating gaps in basic understanding with broad impact
  - Basic understanding enabled by rich data sets and multiscale testbeds
  - Mechanistic understanding, codified in models, supports IAV research
  - Contribute to development of a hi-fidelity national CONUS testbed
  - National testbed can be used to test and validate larger scale models and parameterizations and provide a framework for the integration of local networks

Biological and Environmental Research

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



<u>*Watershed Function and Dynamics: Disturbed & Managed Systems*</u>



SBR Fundamental Research: *BSSD* ⟷ *SBR* ⟷ *CESD*

Goal: Advance a robust predictive understanding of the hydrobiogeochemical structure and function of terrestrial environments from genomes to watersheds

Systems Approach: Iterative, Multi-scale, Interdisciplinary

emergent behaviors

bottom-up — Mechanistic Formulation ⟷ ***Theory*** ⟷ Parsimonious Application — *top-down*

Contributions to CESD, BER and DOE Missions

- Watershed Function and Dynamics – Response to Perturbations
- Contaminant Mobility: plumes to watersheds
- Cycling of Carbon/Critical Elements: microbe-mineral-OM interactions
- Climate Modeling: ESM Grids to Watersheds
- Land-Atmosphere Interactions
  - Plant-Soil-Atm. System to Flux Sites to Watersheds
- Water-Energy-Land Nexus + Mechanistic Foundations for IAV Models

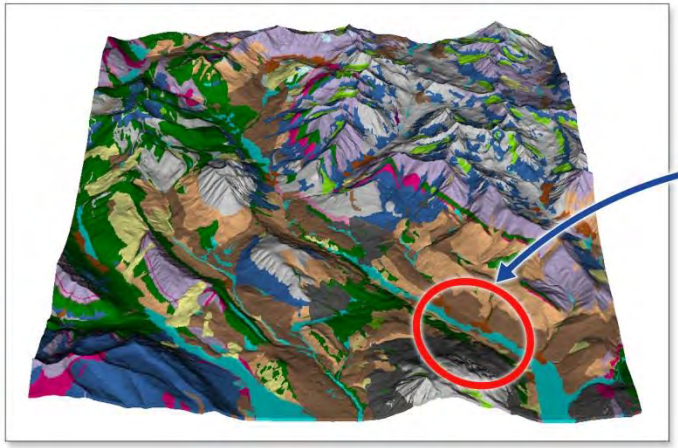
SBR Science Focus Areas

- **LBNL – Watershed Function - Biogeochemical Dynamics from Genomes to Watershed Scales**
  - Model-drive enterprise to develop a predictive understanding of multi-scale, complex, and biologically-based terrestrial environments from genomes to the watershed scale.
- **PNNL – Environmental Significance of the Groundwater-Surface Water Interaction Zone**
  - Developing a predictive understanding of the groundwater-surface water interaction zone and its linkages with the water cycle both in terms of seasonal and annual fluctuations.
- **ORNL – Biogeochemical Transformations at Critical Interfaces**
  - Elucidating the mechanisms by which inorganic Hg is transformed into MeHg at the sediment-water interface and the processes that determine net MeHg production.

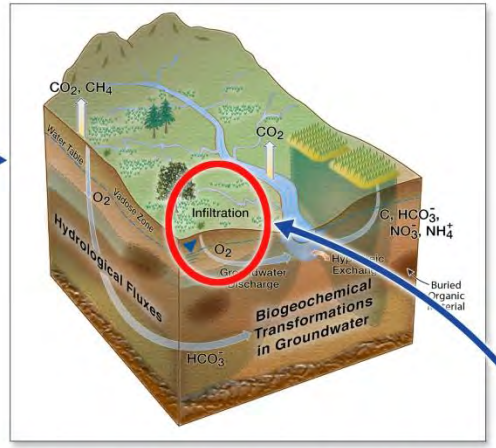
- **ANL – Fe and S Biogeochemistry in Redox Dynamic Environments**
  - Developing understanding of coupled biotic-abiotic molecular- to core-scale transformations of Fe and S within redox-dynamic environments.
- **LLNL – Subsurface Biogeochemistry of Actinides**
  - Identifying the dominant processes controlling actinide transport in the environment.
- **SLAC – Molecular-Scale Biogeochemical Processes Governing the Speciation, Dynamics and Stability of Uranium**
  - Investigating fundamental biogeochemical redox processes that control the behavior of uranium and critical biogeochemical elements.

Building Virtual Ecosystems:

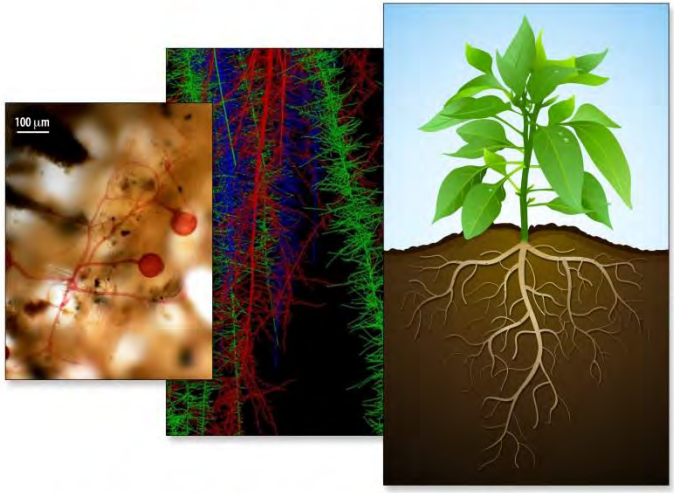
Virtual Plant-Soil System ⇔ Virtual Plot ⇔ Virtual Watershed



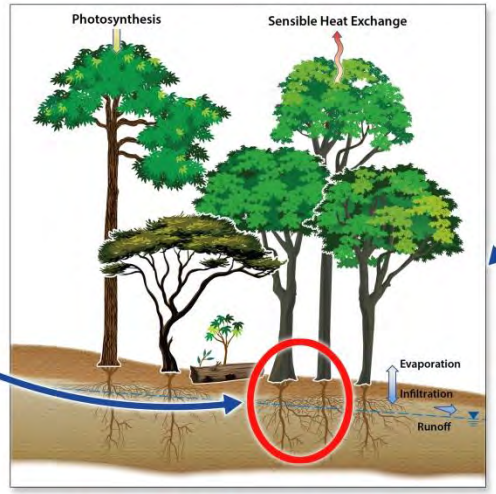
Watershed-scale processes



Catchment-scale hydrology and biogeochemistry



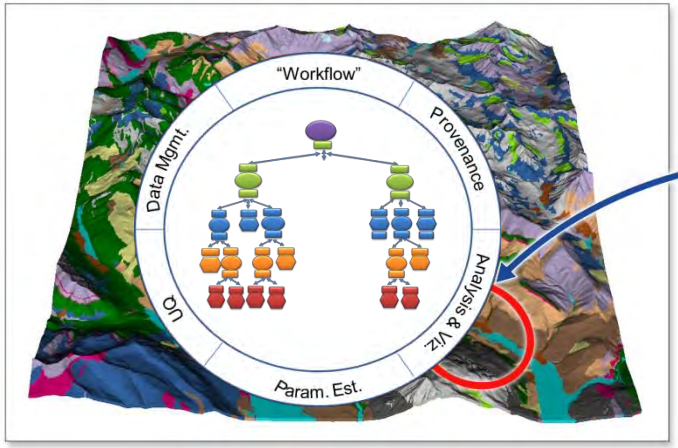
Root interactions with soil and the microbiome



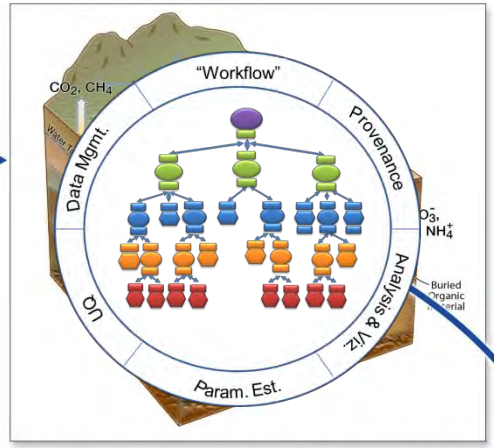
Plot-scale hydrology and vegetation

Building Virtual Ecosystems:

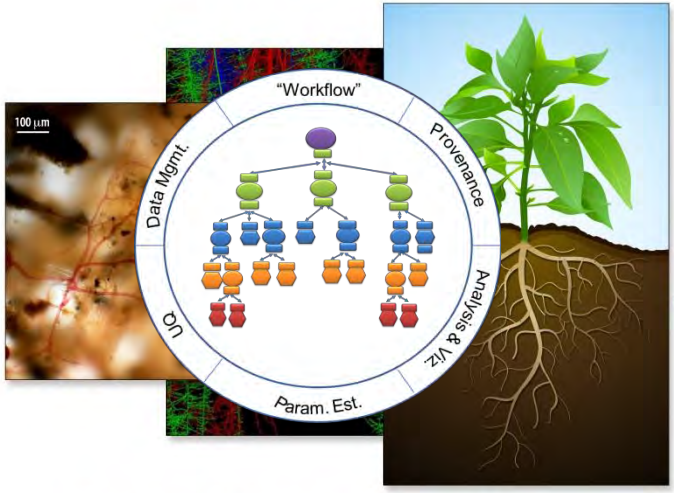
Virtual Plant-Soil System ⇔ Virtual Plot ⇔ Virtual Watershed



Watershed-scale processes



Catchment-scale hydrology and biogeochemistry



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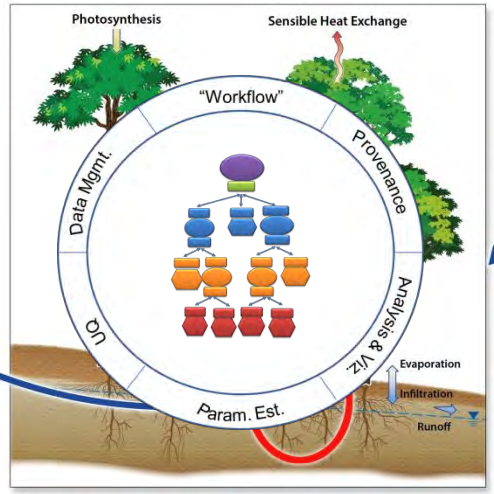
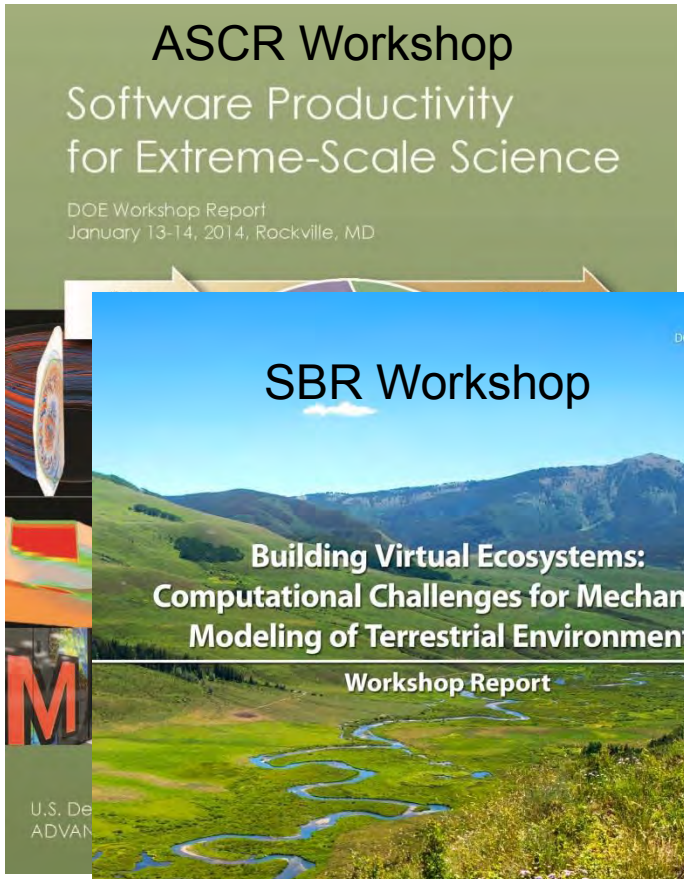
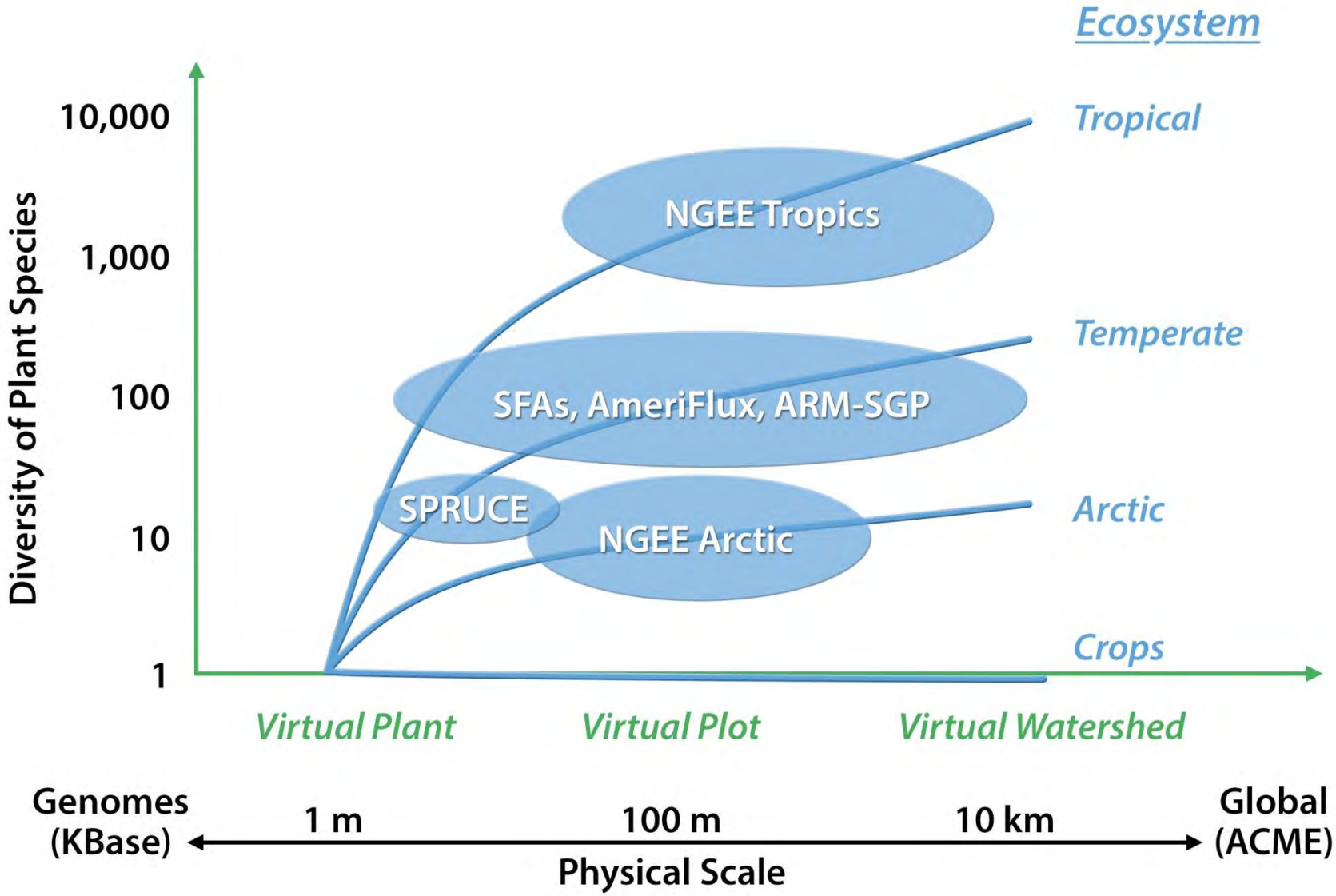


Plot-scale hydrology and vegetation

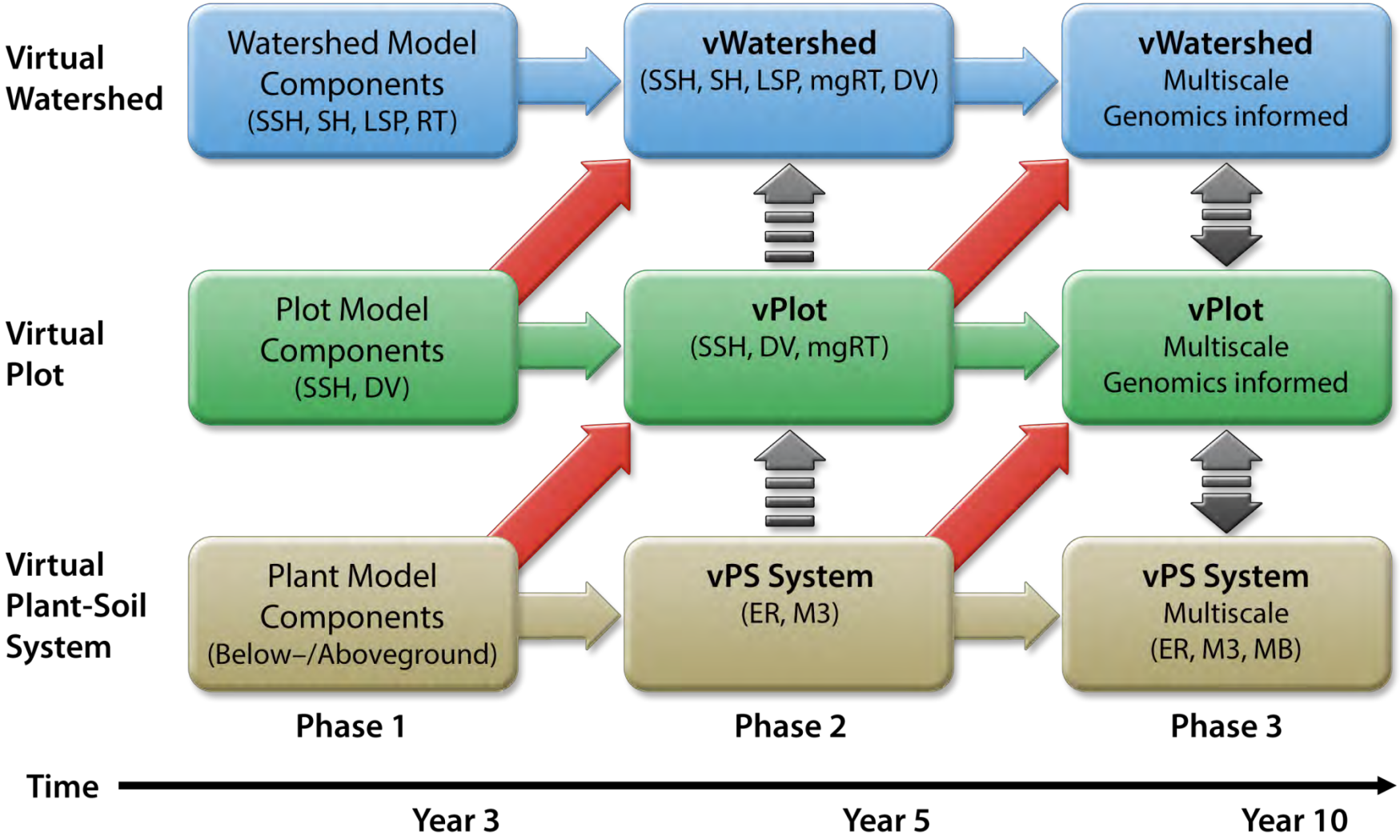
Most Recent Workshops



CESD Field Research Activities



Integrated Software Ecosystem
Phased Approach to Science-Driven Co-Development



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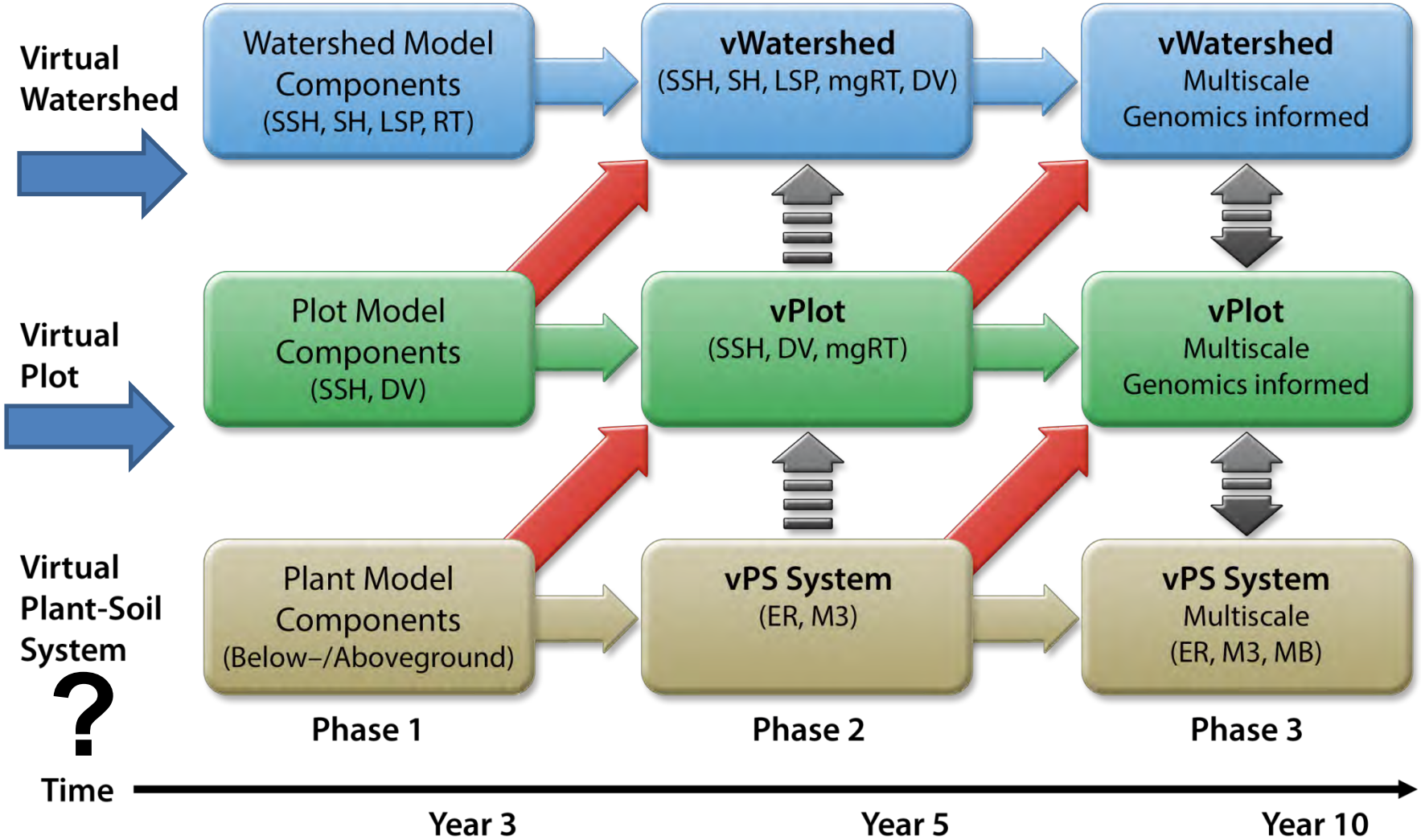


Virtual Plant-Soil System: *Why and How?*

Natural Ecosystems

- Develop more realistic plant-functional-types in ESMs (<20 PFTs in current GCMs)
- Develop mechanistic basis for extrapolating plant structure-function relationships to future climate states using PFTs and trait-based models (e.g., drought, temp. , CO_2, etc.)

Sustainable Bioenergy Feedstocks

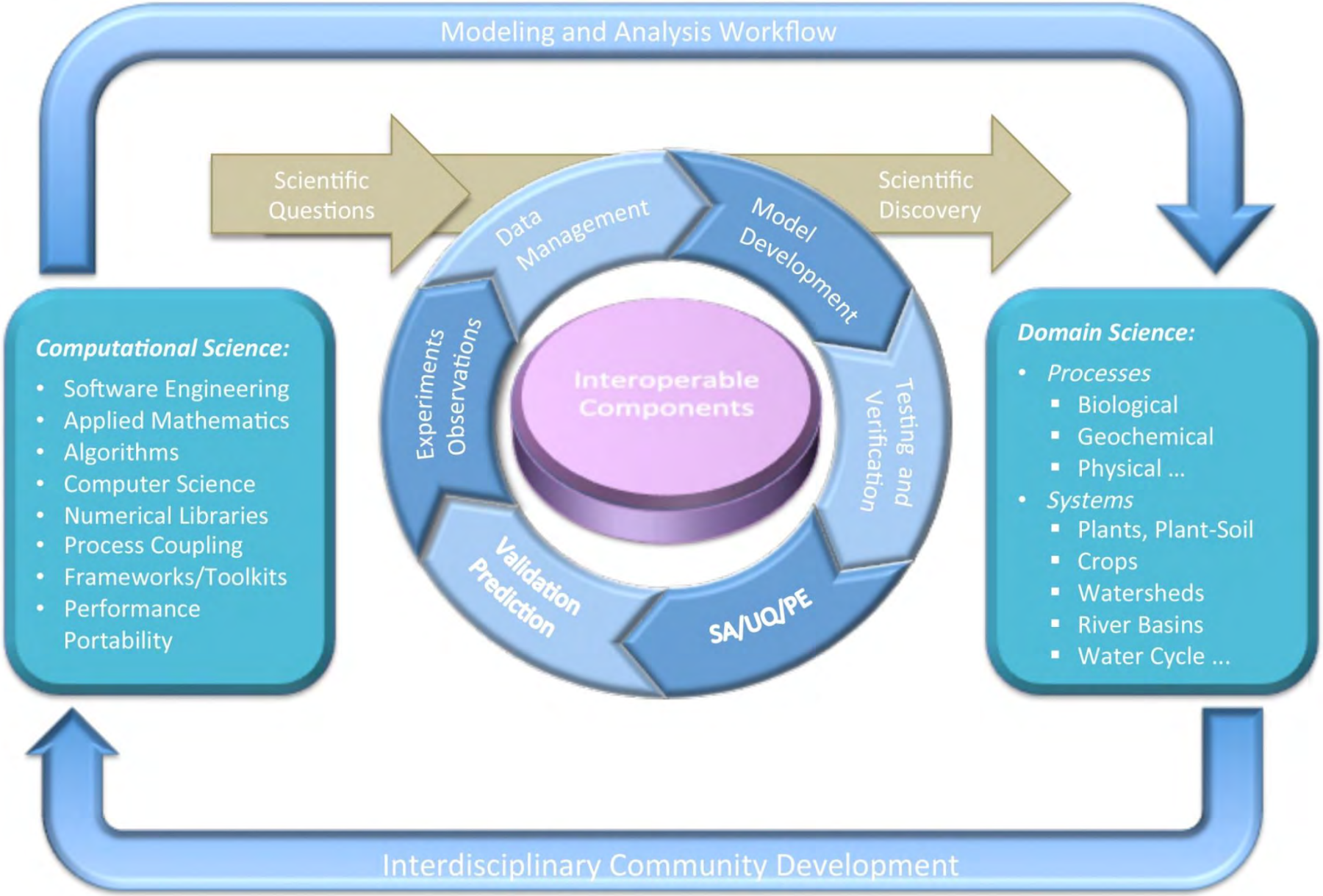
- Provide integrative framework for understanding plant-soil systems where implications for discovery at smaller scales (e.g., root-microbe interactions) can be examined at whole plant and crop scales => *Support hypothesis generation and testing*
- Allow the application of optimization algorithms to identify more resource efficient ideotypes to guide breeding of emerging sustainable bioenergy crops: GxExM

Phased Approach to Development: *Design, Build, Test, Learn*

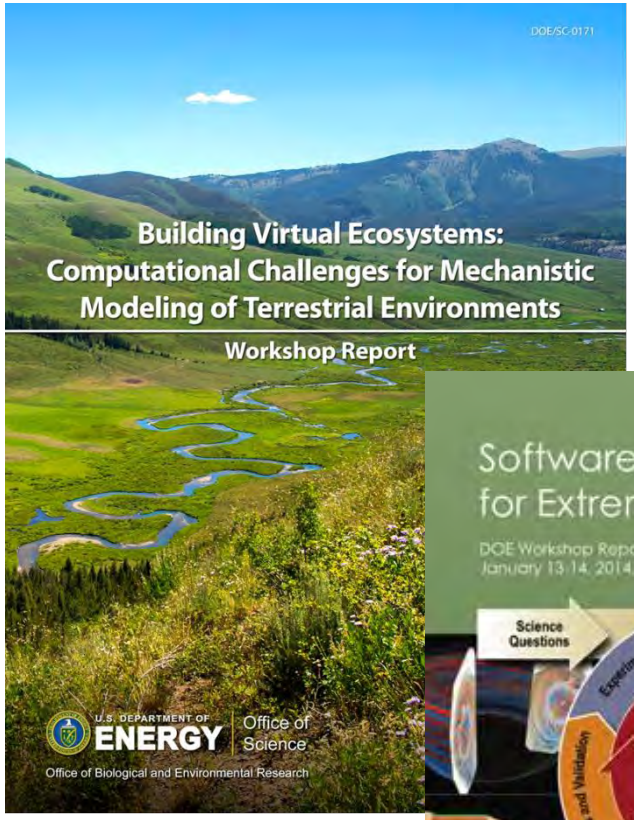
- Integrate isolated models of plant components and processes to develop a framework to mechanistically capture the structure and function of whole plant-soil systems
- Start with biophysical models of 1 to 2 herbaceous bioenergy crop monocultures ("model organisms") with robust aboveground and belowground plant components coupled to reactive transport models of soil (including microbiome genomics)
- Compelling science questions drive an iterative cycle of co-development and testing to increase model fidelity and range of species
- Incorporate plant and microbial genomic information

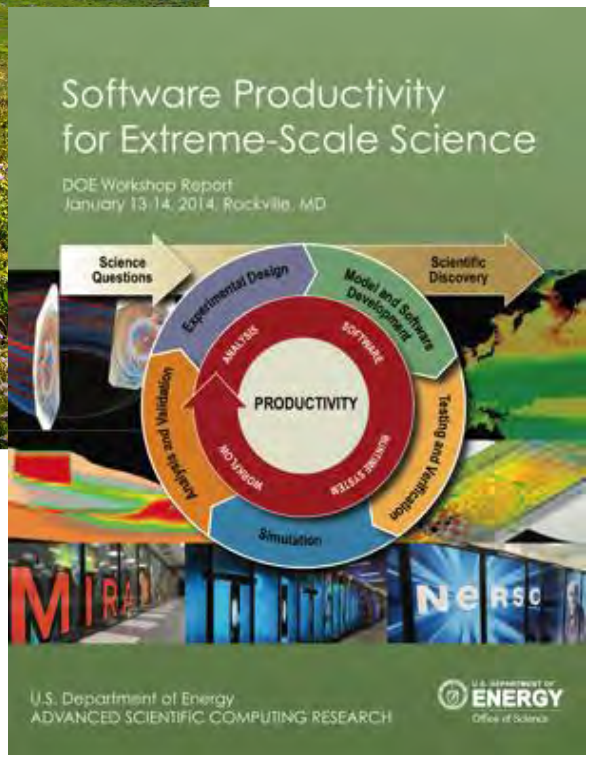
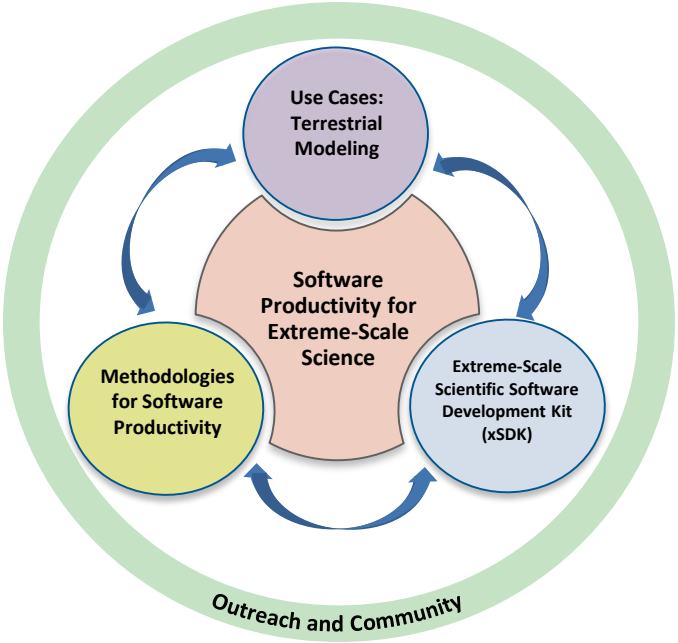
Integrated Software Ecosystem

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



DOE ESS and ASCR Workshops catalyzed a collaborative project on Software Productivity





IDEAS productivity