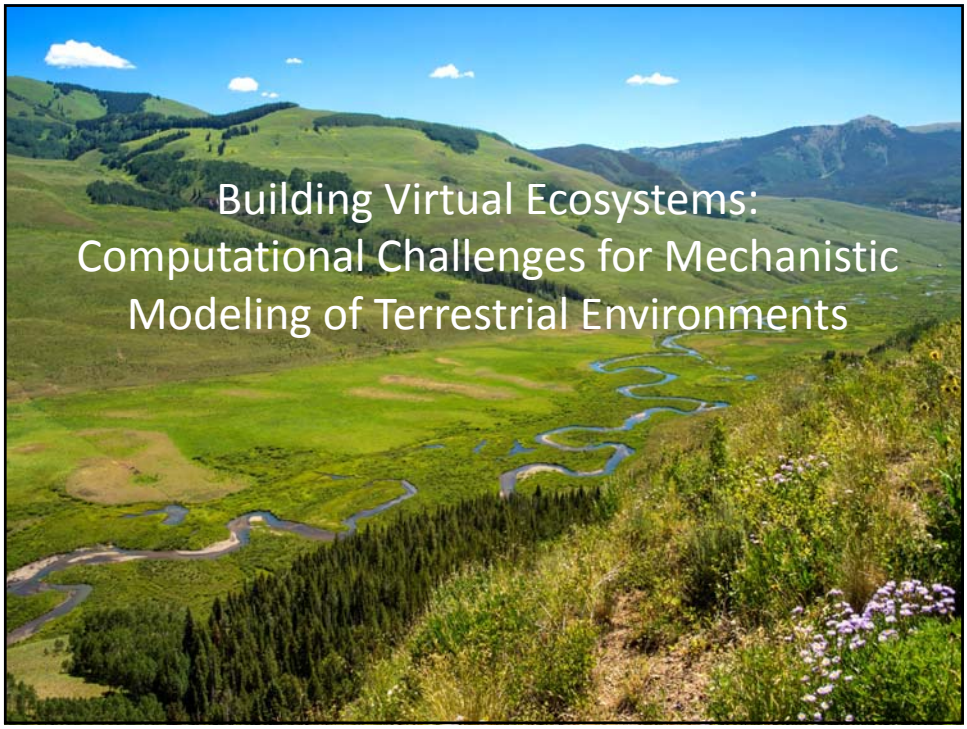


Building Virtual Ecosystems: Computational Challenges for Mechanistic Modeling of Terrestrial Environments

The Challenges:

- ***Complexity:*** seek to understand and predict the structure and function of complex terrestrial environments across vast spatial and temporal scales
- ***Fragmentation:*** Require a more seamless modeling framework.
- ***Disruptive Hardware:*** legacy codes built to run on computers composed of single-processors will not run efficiently on heterogeneous computer architectures of the near future (HPC to PC).

Workshop Scope:

- Develop design requirements, principles for governance and a phased approach for building a community modeling framework to advance a mechanistic, multiscale and multiphysics understanding of complex terrestrial environments extending from plants to plots to watersheds and beyond…

Workshop details

Germantown, MD
March 26-27, 2014

- Leadership:

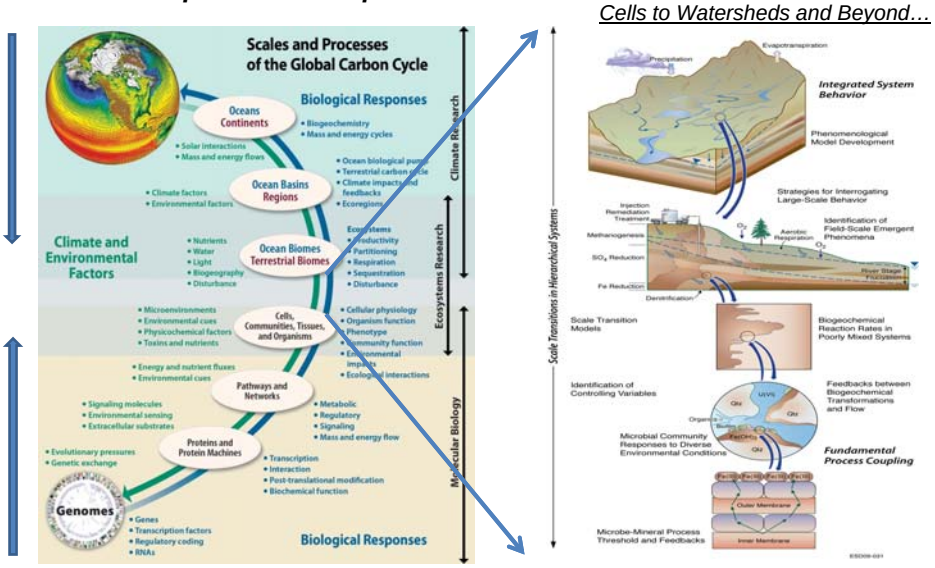
PM's	• David Lesmes (BER) • Paul Bayer (BER)
RTM/ Hydro	• Dave Moulton (LANL): co-org • Tim Scheibe (PNNL): co-org • Carl Steefel (LBNL): co-org • Scott Painter (ORNL)
ESM	• Peter Thornton (ORNL) • Charlie Koven* (LBNL)
Plants	• Stephen Long (UIUC) • Jonathan Lynch (PSU)
Genomics	• Eoin Brodie (LBNL) • David Weston (ORNL)
CS/SE	• Mike Heroux (SNL) • Lois Curfman McInnes (ANL)

- Participants:
  - David Bernholdt (ORNL)
  - Anthony Bishopp (U. Nottingham, UK)
  - Valentin Couvreur, (UC Davis)
  - Scott Denning (Colorado St. U.)
  - Darren Drewry (JPL–NASA)
  - Chris Duffy (Penn. St. U.)
  - Michael Ek (NOAA)
  - Glenn Hammond (SNL)
  - Kerstin Kleese van Dam (PNNL)
  - Paul Moorcroft (Harvard U.)
  - Gretchen Miller (Texas A&M U.)
  - Amilcare Porporato (Duke U.)
  - Lawren Sack (UCLA)
  - Shawn Serbin (BNL)
  - Elena Shevliakova (NOAA)
  - Dali Wang (ORNL)
  - John Wu (LBNL)
  - Xinguang Zhu (Shanghai Inst. of Sci.)

Biological and Environmental Research

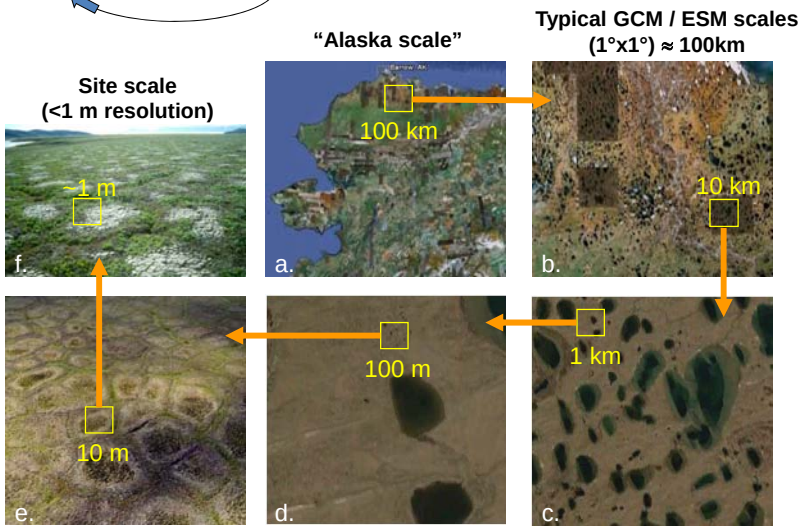
Understanding complex biological, climatic, and environmental systems across vast spatial and temporal scales

Cells to Watersheds and Beyond…



EXAMPLE *Multiscale-Multiphysics* System: Arctic Tundra

Models + Data (Obs/Exp) => Predictive Understanding

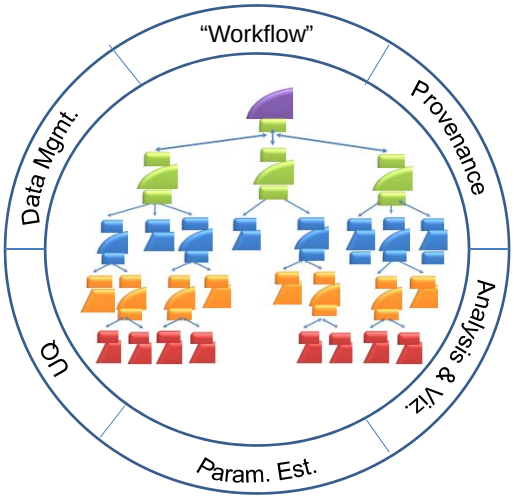


Landscape scales (100 m to 10 km)

Integrated Software Ecosystem

Multiscale-Multiphysics Framework: Modular, interoperable, extensible, agile and easy to use across platforms (HPC to PC)

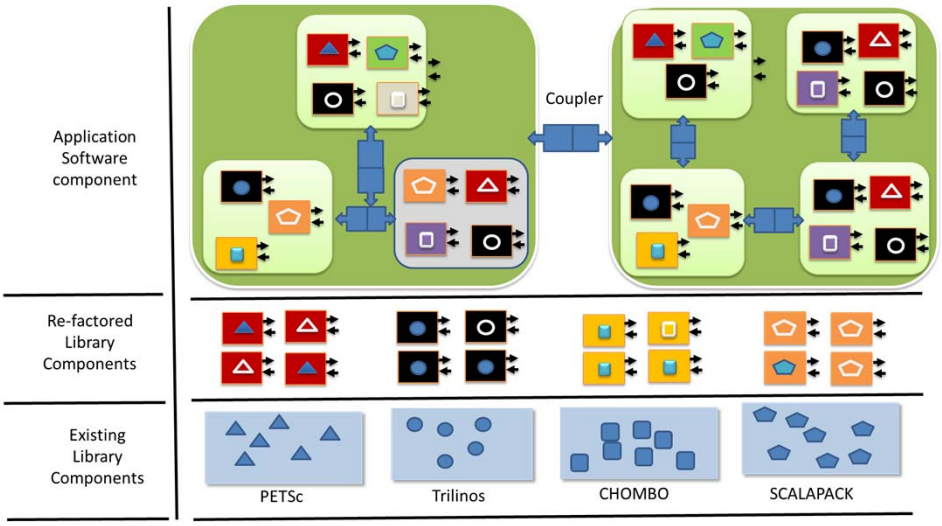
Computer Science:
-Software Eng.
-Applied Math
-Libraries
-Couplers
-Etc…



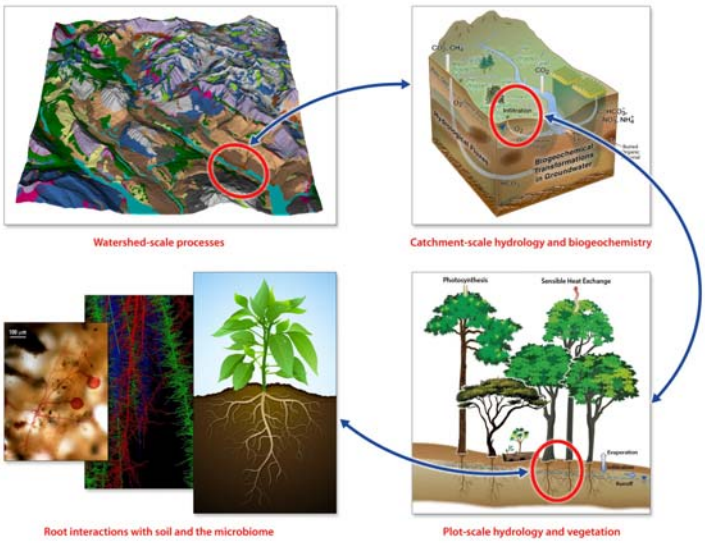
Domain Science:
Systems:
-Plants
-Crops
-Watersheds
-River Basins
-iH_2O Cycle
-Etc…

Processes:
Phy⇔Chm⇔Bio

Integrated Software Ecosystem:
A *Computer Science Grand Challenge*



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



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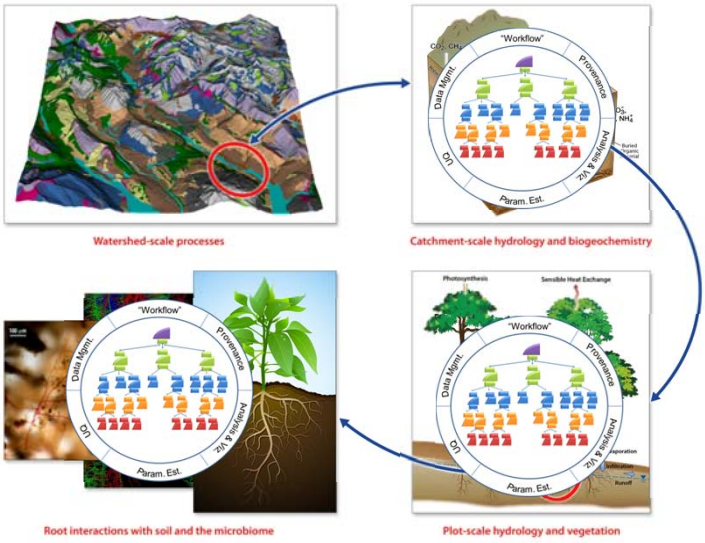
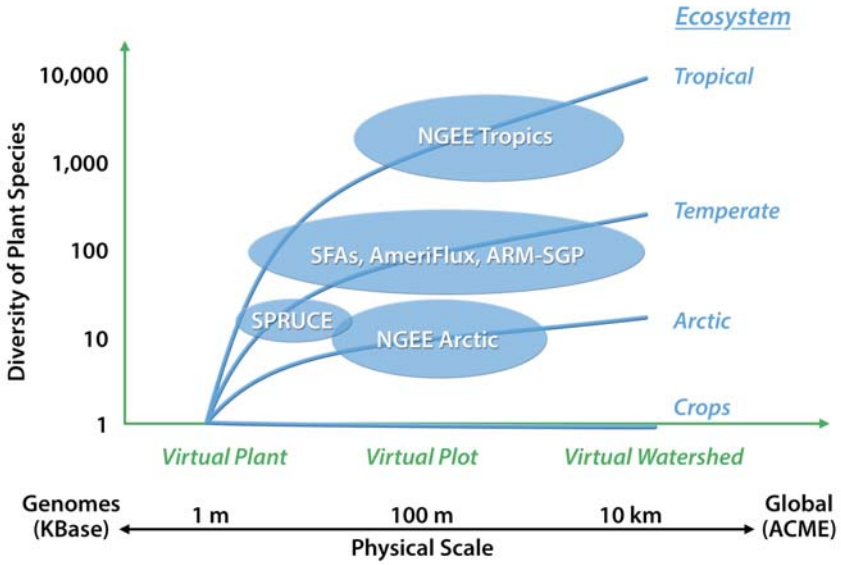
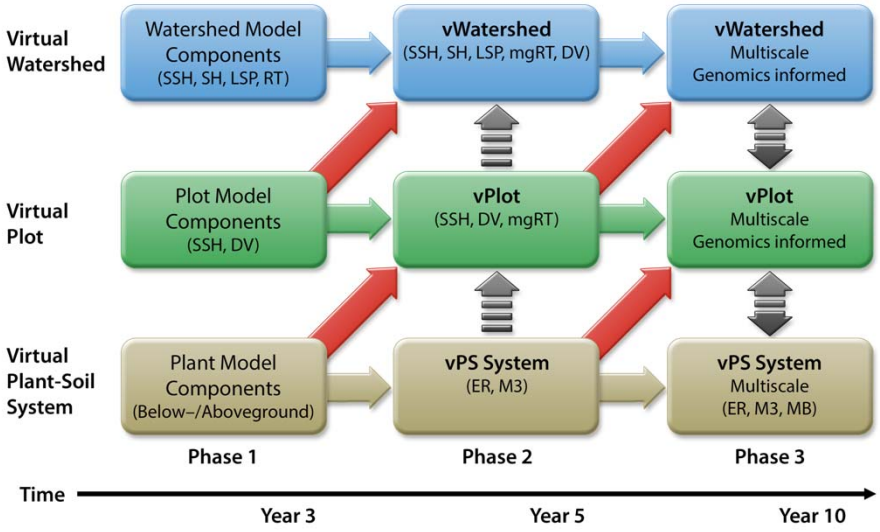


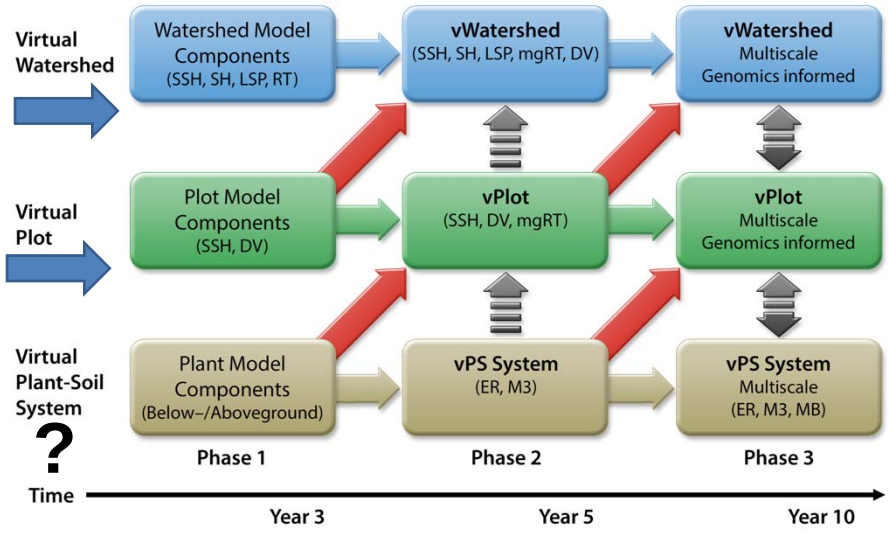
CESD Field Research Activities



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



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



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

Workshop Outcomes

- Workshop report on BER website
  http://doesbr.org/VirtualEcosystems/
- IDEAS Productivity project, supported by ASCR and BER
  https://ideas-productivity.org/
- Environmental System Science (ESS) Working Group being developed on Model-Data Integration
  - Modeling Frameworks + Data Management and Workflows + Software Engineering
- Two publications from the workshop discussions
  - "Plants in Silico", Long, Zhu, Stitt, Millar, Lynch and LeBauer, Plant, Cell & Environment (PCE), accepted
  - "Virtual Watersheds," in preparation

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***

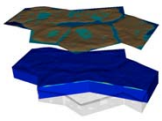
Objectives

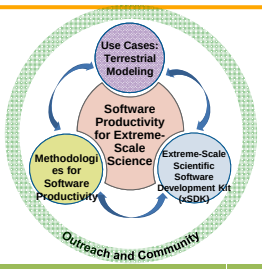
Address confluence of trends in hardware and increasing demands for predictive multiscale, multiphysics simulations.

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)

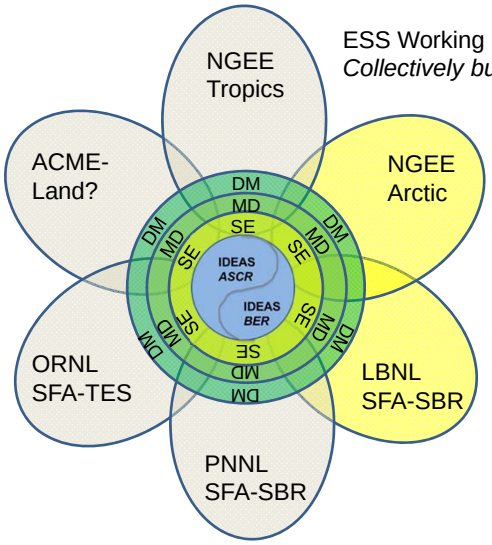
BER Lead: David Moulton (LANL)

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/

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



ESS Working Group: Model-Data Integration
Collectively building "MODEX" capabilities

ESS Working Group Teams

- Software Engineering (SE)
- Model Development (MD)
- Data Management (DM)

Project	SE	Mod	DM
IDEAS			
NG-A			
LBNL			
NG-T			
PNNL			
ORNL			
ACME-L			

Integrated Software Ecosystem

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