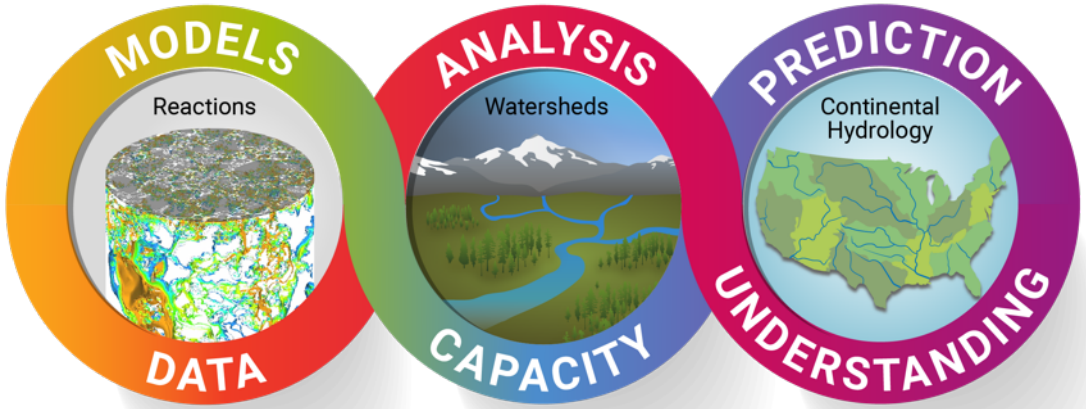
IDEAS-Watersheds

Accelerating watershed science through a community-driven software ecosystem



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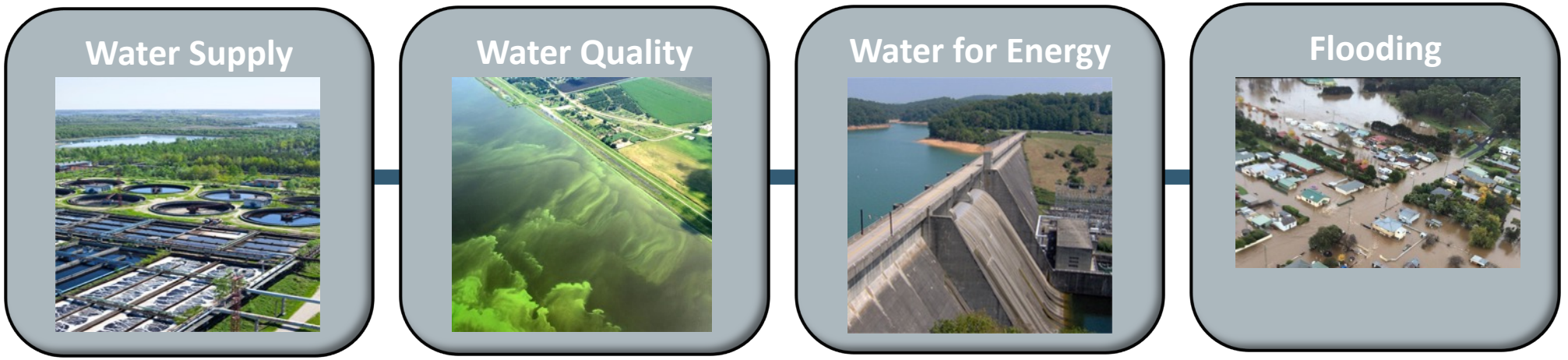
U.S. DEPARTMENT OF ENERGY | Office of Science

https://ideas-productivity.org/ideas-watersheds

Argonne NATIONAL LABORATORY | BERKELEY LAB | Lawrence Livermore National Laboratory | Los Alamos NATIONAL LABORATORY EST.1943 | OAK RIDGE National Laboratory | Pacific Northwest NATIONAL LABORATORY | ARIZONA | NCAR | SCHOOL OF MINES 1874 COLORADO

Healthy Watersheds: Critical to Water Security

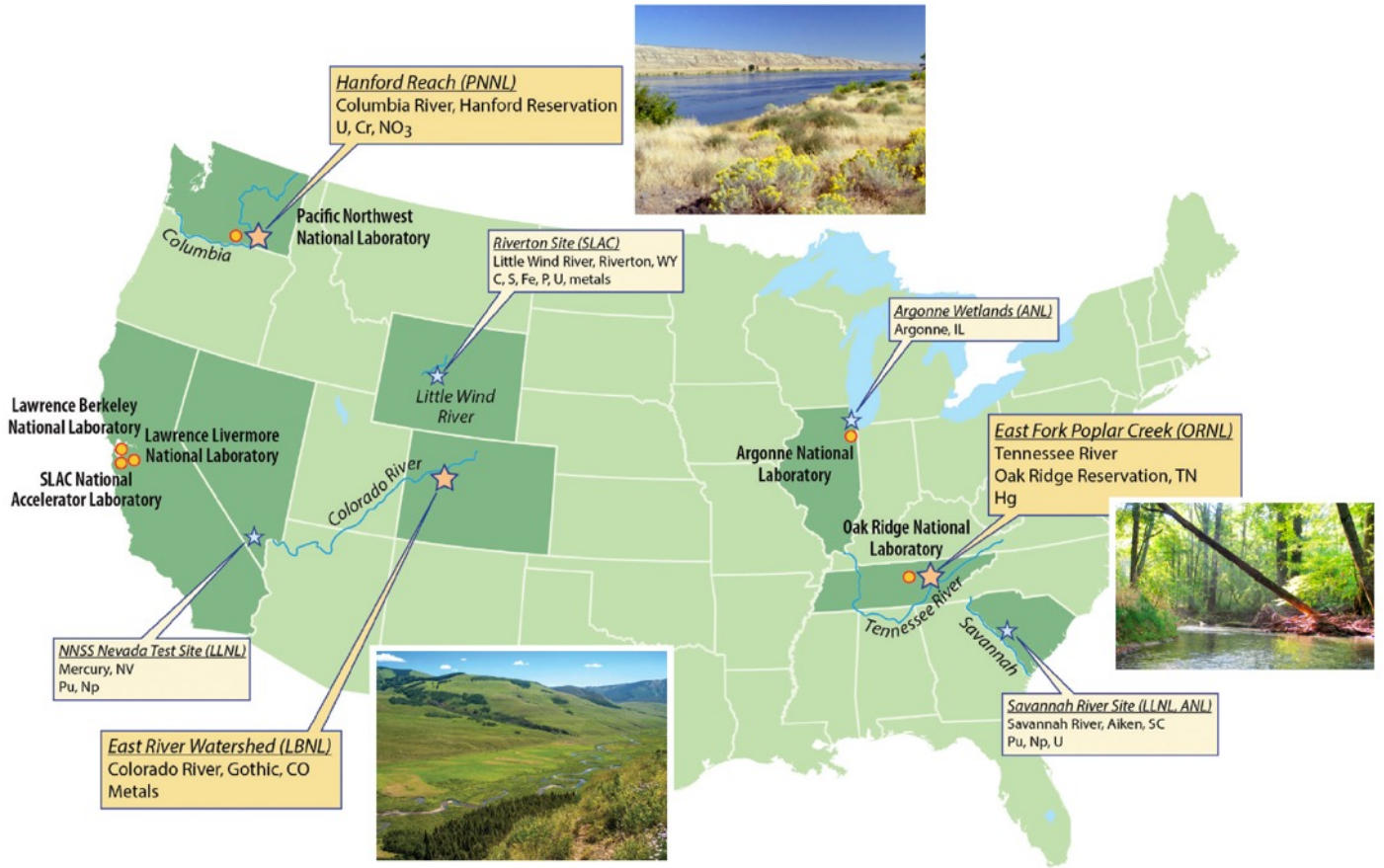


- Watersheds protect the Nation's water supply by
  - Buffering precipitation inputs
  - Filtering sediments
  - Biogeochemically transforming contaminants and excess nutrients
- Watershed function is stressed by global change
  - Increases in contaminant and nutrient inputs
  - Changing precipitation patterns, land use, and temperature

IDEAS WATERSHEDS

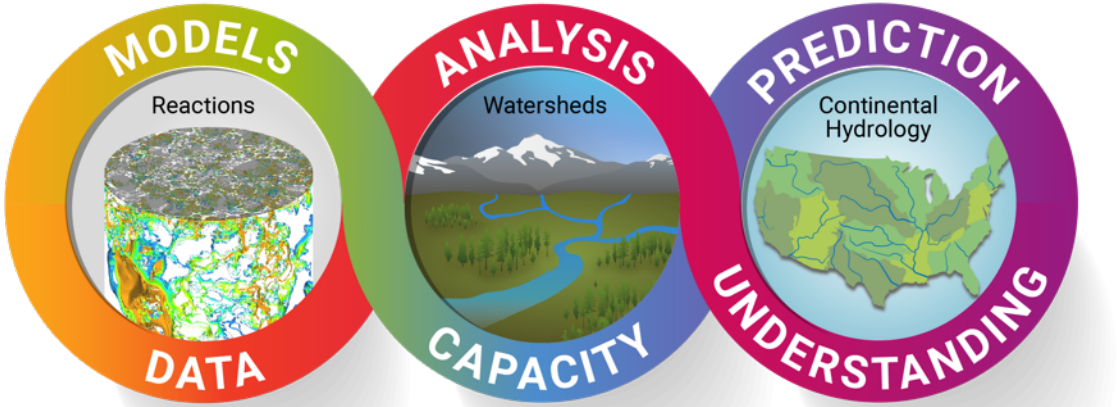
SBR Seeks a Robust Predictive Understanding of Watershed Hydrobiogeochemical Function

- Unique capabilities
  - Biogeochemistry
  - Microbial processes
  - Integrated flow and reactive transport modeling
  - Model/data integration
  - High-performance computing
- Interdisciplinary distributed watershed testbeds



IDEAS WATERSHEDS

IDEAS-Watersheds Confronts the Central Challenges in Computational Watershed Science



- Enable SBR scientists to represent effects of fine-scale biogeochemical process understanding in models that address societally relevant scales
- Improve interoperability among existing tools and advance new community capabilities to expose untapped synergies across projects.
- Realize the potential of DOE's high-performance computing resources by improving software design and engineering practices.
- Develop multiscale model-data integration and analysis workflows that leverage rapidly growing and diverse data sources.

IDEAS WATERSHEDS

IDEAS productivity
www.ideas-productivity.org

Interoperable Design of Extreme-scale Application Software (IDEAS)

MISSION STATEMENT

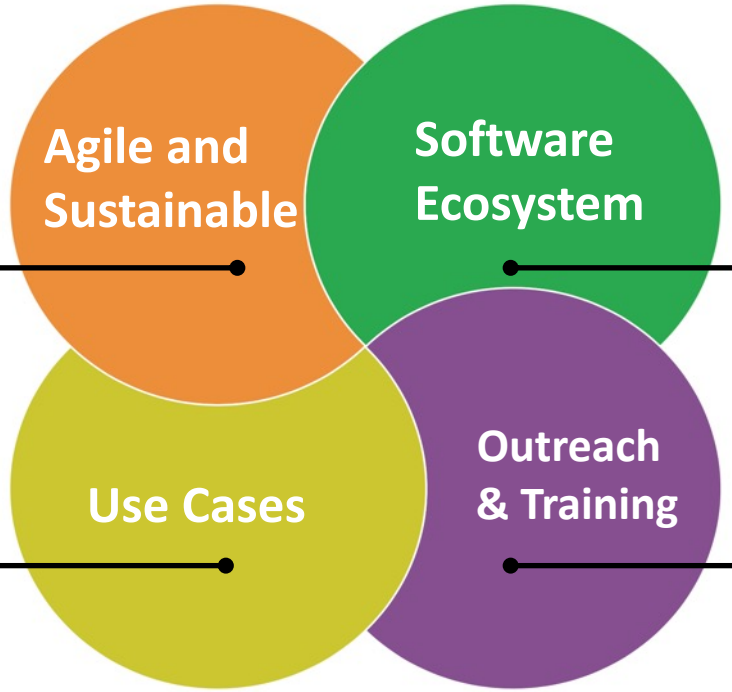
Increase scientific productivity by improving software, advancing community shared capabilities, and realizing the potential of advanced computing resources.

BACKGROUND

IDEAS Family of synergistic projects: IDEAS-Classic (the original ASCR/BER partnership) has launched two Exascale Computing Program (ECP) projects. IDEAS-ECP and xSDK4ECP. and IDEAS-Watersheds (proposed).

APPROACH

Promote agile software engineering methodologies and improved design.



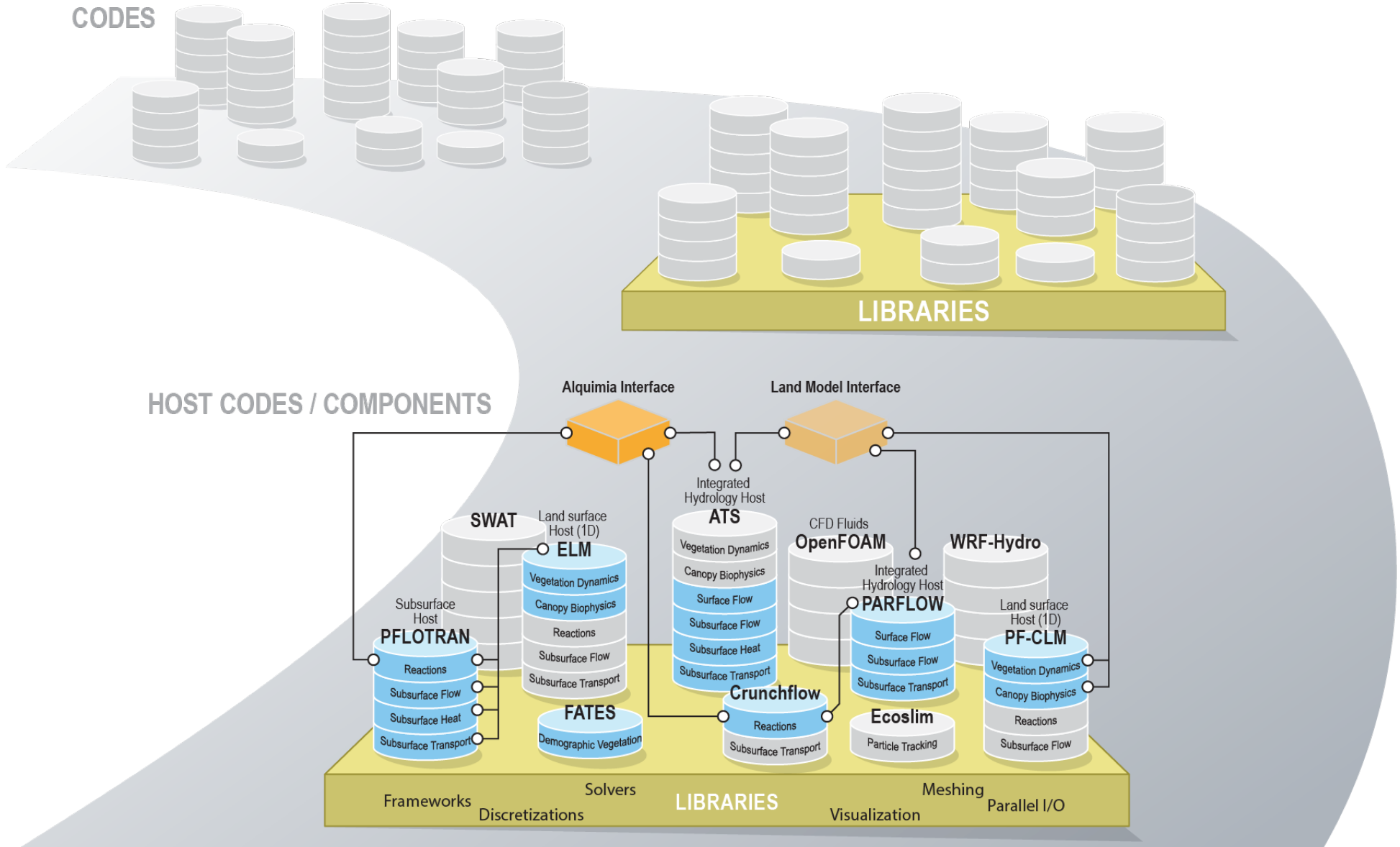
Advance the community software ecosystem of interoperable components

Create **partnerships** between IDEAS and SFAs centered on concrete Use Cases with shared deliverables.

Train team of postdocs as interdisciplinary computational scientists and **liaisons.**

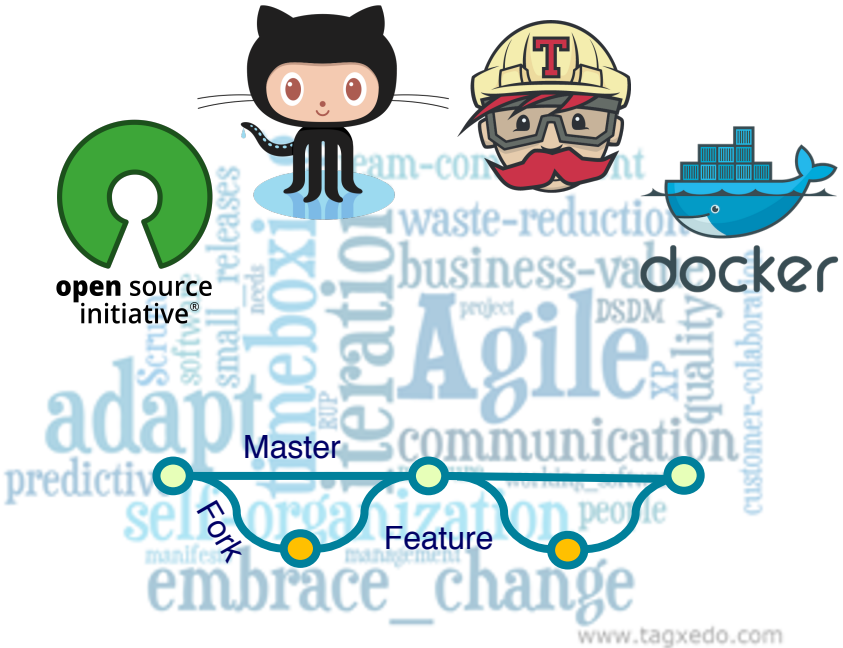
IDEAS-Watersheds Software Ecosystem

From Silos to an Ecosystem



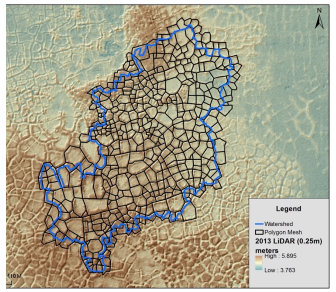
xSDK includes the Libraries, Interface Libraries, and interoperable components.

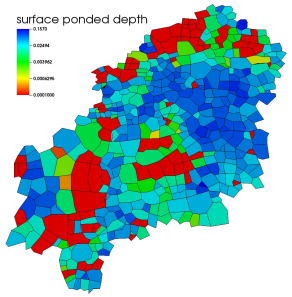
Agile Tools, Methodologies and Use Cases

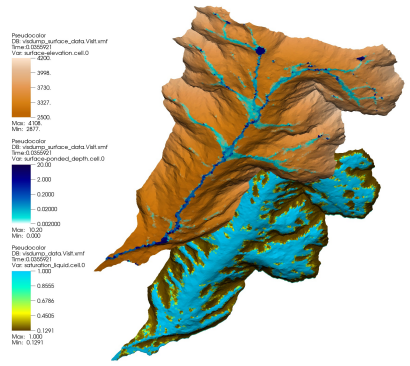


http://agilemanifesto.org

Tools and Methodologies ensure developer productivity of open, sustainable, flexible, and portable software ecosystem.







Use Cases connect to science challenges, ensure effectiveness and transferability.

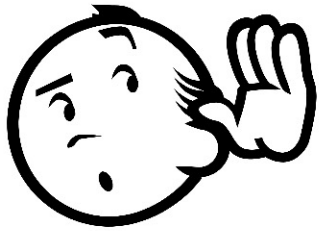
Developing IDEAS-Watersheds we realized we were still missing something?

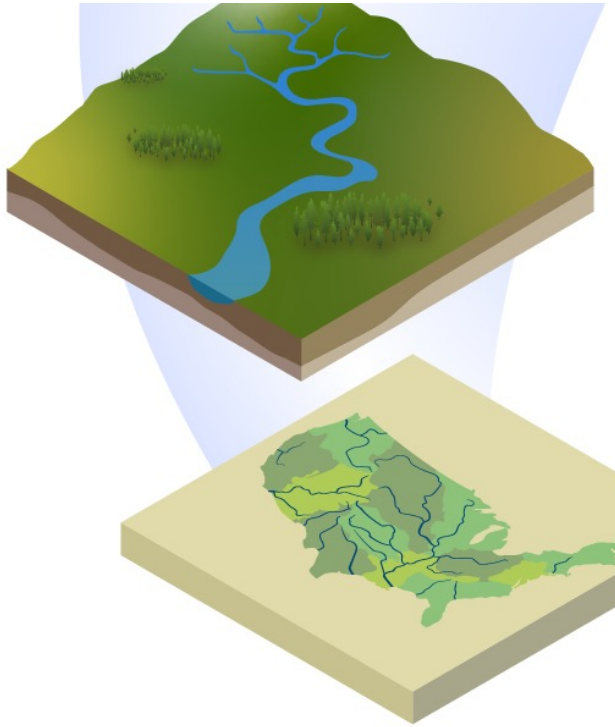
IDEAS WATERSHEDS

IDEAS-Watersheds Activities

Develop Use Case Concepts for the additional SFAs.

- Build on lessons learned from the “Collaborative Design Challenge” at 2018 CI WGs Annual Meeting





Watershed hydrobiogeochemistry

Scaling to watersheds

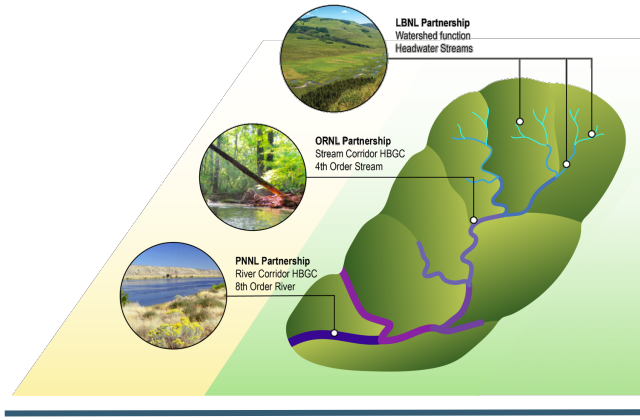
- Hydrological exchange flows and biogeochemical processes interact to control system function
- Advance stream and river corridor frameworks

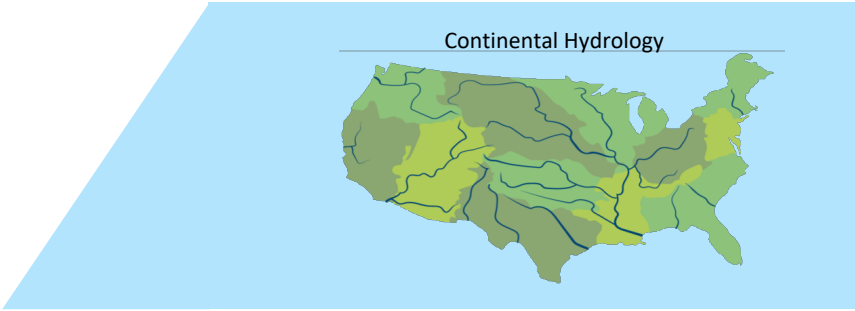
Basin to continental hydrology

Connecting across watersheds

- Hydrological context for SFA testbeds
- Infrastructure for upscaling

ANL, LLNL, SLAC?

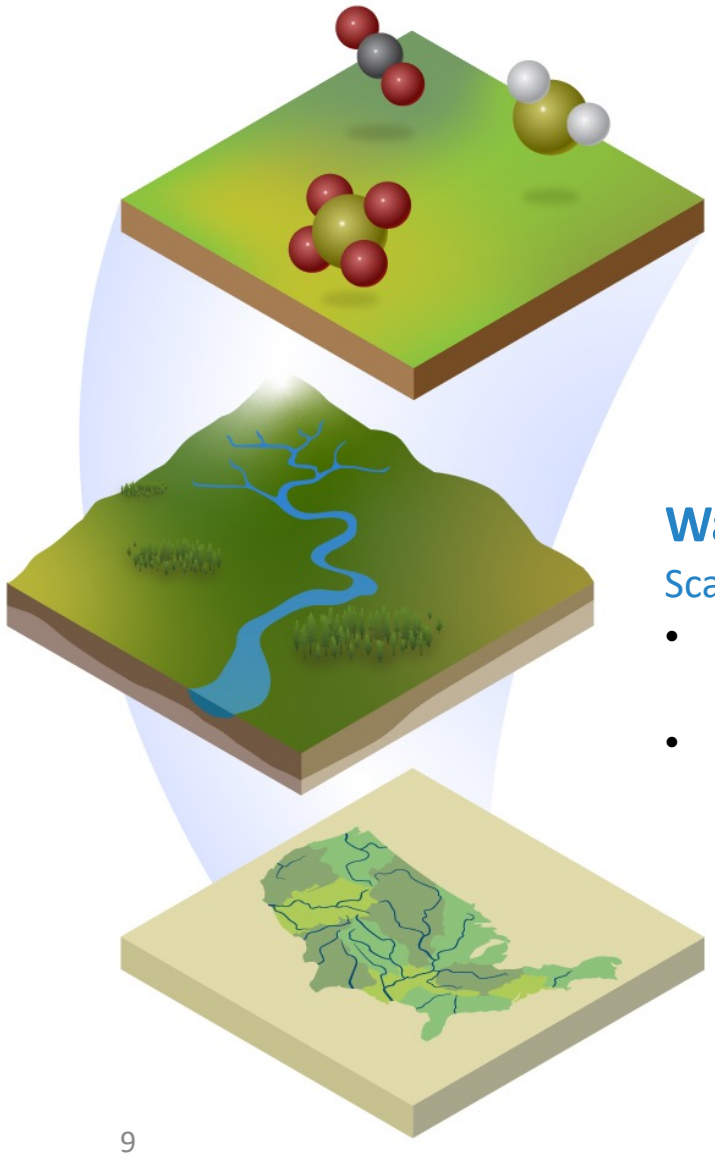




IDEAS-Watersheds Shared Infrastructure

IDEAS WATERSHEDS

IDEAS-Watersheds Activities



Reactions

Biogeochemical reaction networks

- Enhance capabilities of geochemistry engine
- Leverage genomic and molecular advances, e.g.
  - DOE Systems Biology Knowledgebase (KBase)
  - DOE Environmental Molecular Sciences Laboratory (EMSL)
- Improve interoperability by advancing Alquimia interface library

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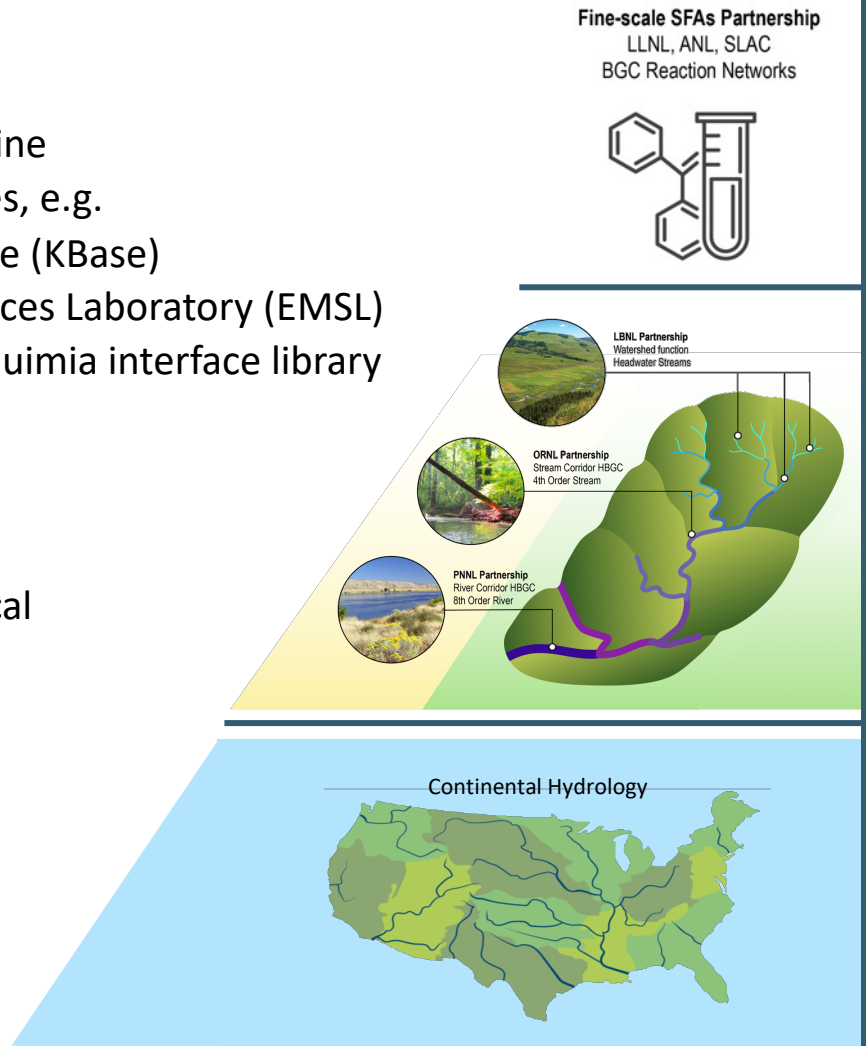
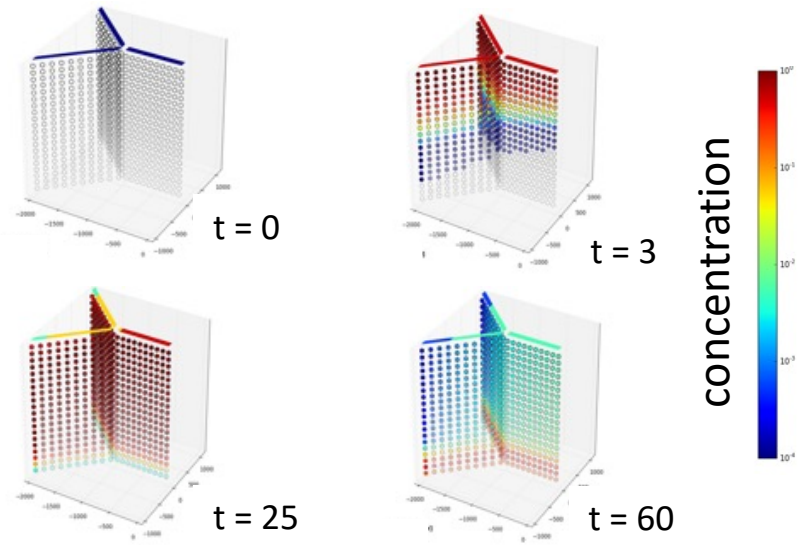


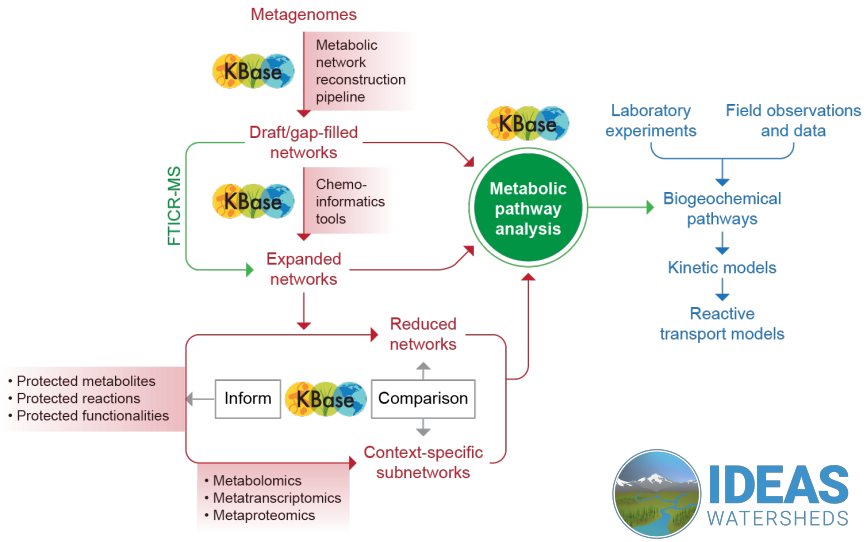
IDEAS-Watersheds Shared Infrastructure

IDEAS WATERSHEDS

IDEAS-Watersheds Recent Research Activities

- Watershed Function SFA: East River Use Case.
  - Developing and demonstrating an integrated hydrology (coupled surface/subsurface) reactive transport capability
- River Corridor SFA: Columbia River Use Case
  - Modeling pipeline from metagenomes to biogeochemical models to reactive transport leveraging the KBase platform
- Critical Interfaces SFA: East Fork Popular Creek Use Case
  - Developing and demonstrating multiscale model of hyporheic exchange as a subgrid process leveraging travel times.
- CONUS
  - Completed warming study on the first generation domain, demonstrating significant impact of evapotransporation depleting groundwater (Condon et al. Nat Commun, 2020)

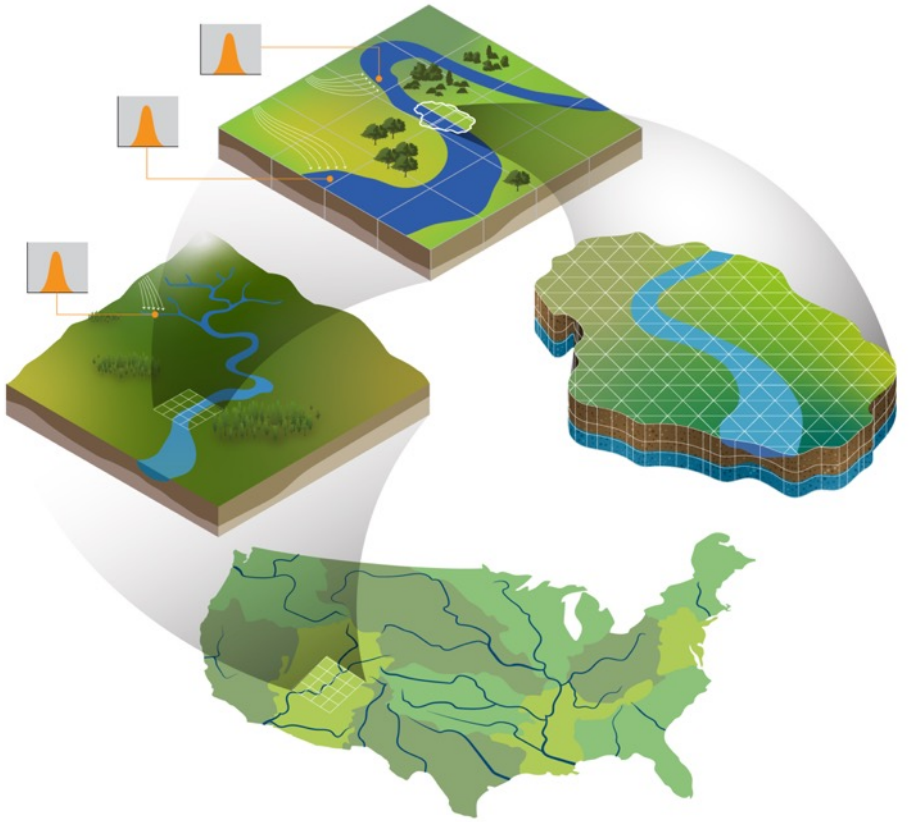




IDEAS WATERSHEDS

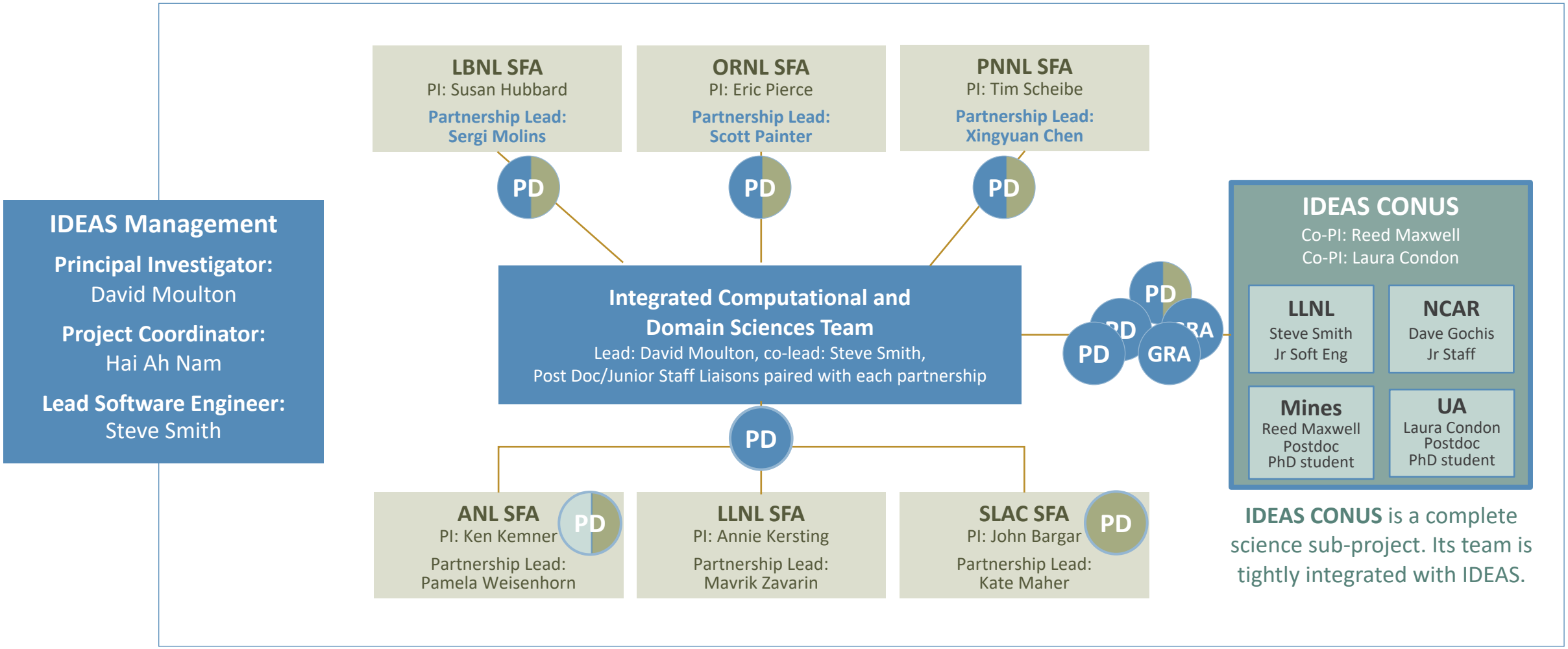
IDEAS–Watersheds: Shared Infrastructure

- Multiscale Meshing Workflows
  - Subsetting coarser-resolution model outputs as inputs to higher-resolution models
  - Tools for constructing multiresolution unstructured meshes that capture river corridors
- Interfaces
  - Improve Alquimia, and add support for PHREEQc
  - Explore interface design for Land Models, including plant models and coupling.
  - Prototype interface with PF-CLM, document requirements of fine-scale integrated hydrology.
- Sustainable Software Ecosystem
  - Develop a central web presence
  - Develop more formal guidelines for growth and support of ecosystem codes based on xSDK policies.
  - Contribute domain libraries to the xSDK



IDEAS WATERSHEDS

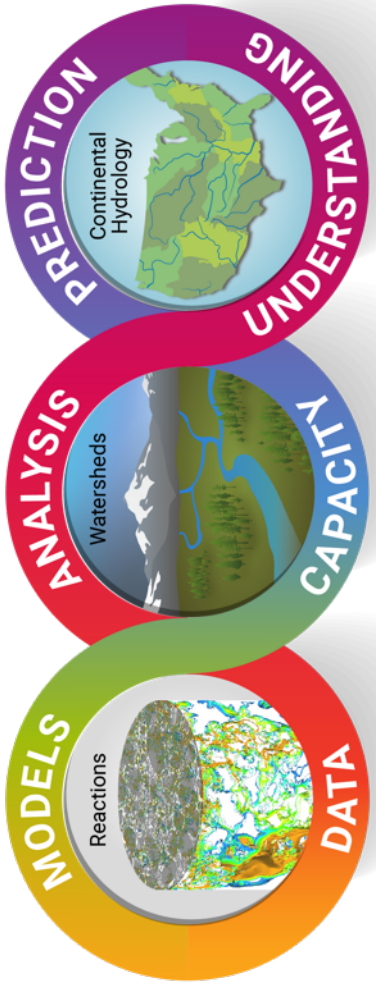
IDEAS-Watersheds: Integration



IDEAS-Watersheds

Integrate and broaden the impact of the SBR cornerstones and testbeds

- Enhance productivity in watershed science.
- Create a more viable software ecosystem through the SFA Partnerships to bring broader science impact to the community.
- Bridge fine-scale mechanistic models and studies to regional and climate relevant scales through CONUS Activities & leadership.
- Provide outreach & engage the broader community and leverage resources for inter-agency efforts at a range of scales.
- Train a wave of skilled young computational scientists geared toward interdisciplinary teams and adaptable sustainable software.



IDEAS WATERSHEDS