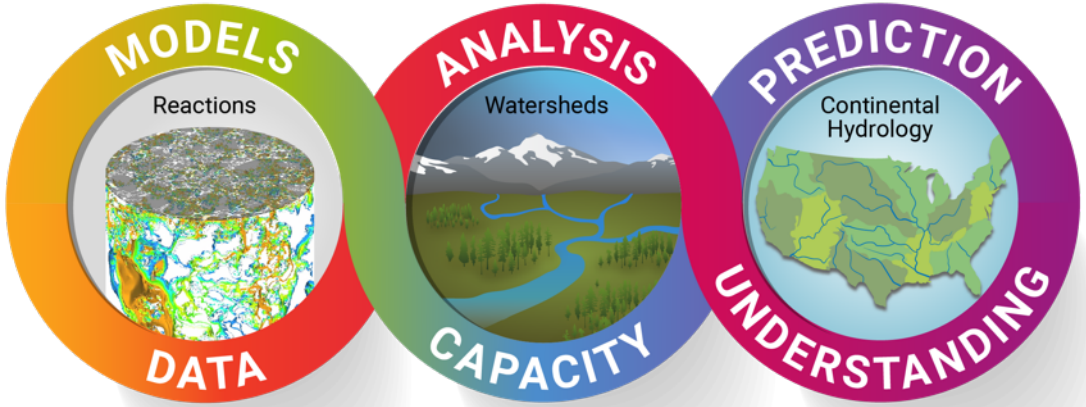
# IDEAS-Watersheds

## Productivity and Sustainability in a Community-Driven Software Ecosystem for Watershed Science




Office of Biological and Environmental Research (BER)
Subsurface Biogeochemsitry Research (SBR) program


**PI:** David Moulton (LANL)

**Activity Leads:**

Sergi Molins (LBNL)
Scott Painter (ORNL)
Xingyuan Chen (PNNL)
Laura Condon (UA)
Reed Maxwell (Mines)

**Software Lead:**

Steve Smith (LLNL)

**Project Coordinator:**

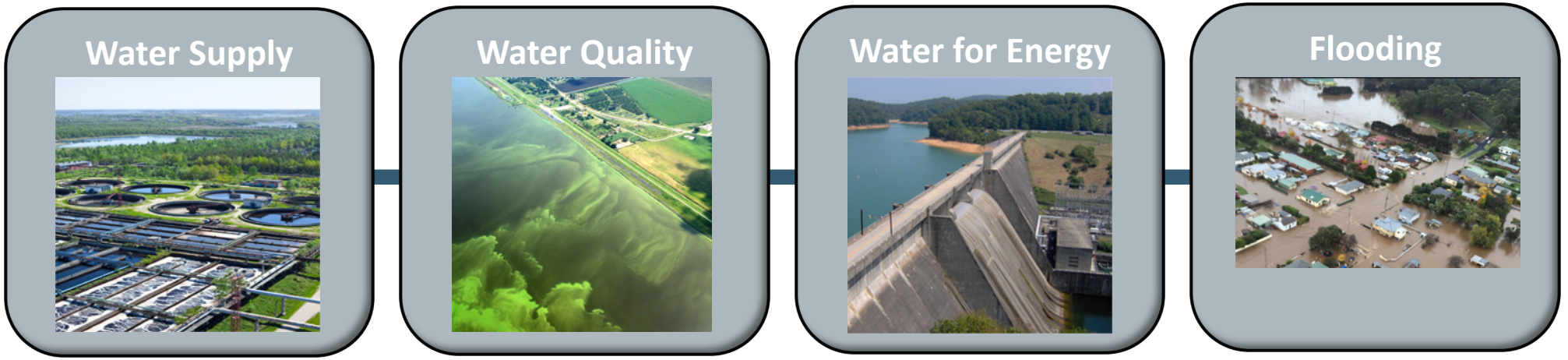
Hai Ah Nam (LANL)


U.S. DEPARTMENT OF ENERGY | Office of Science

LA-UR-20-21425

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

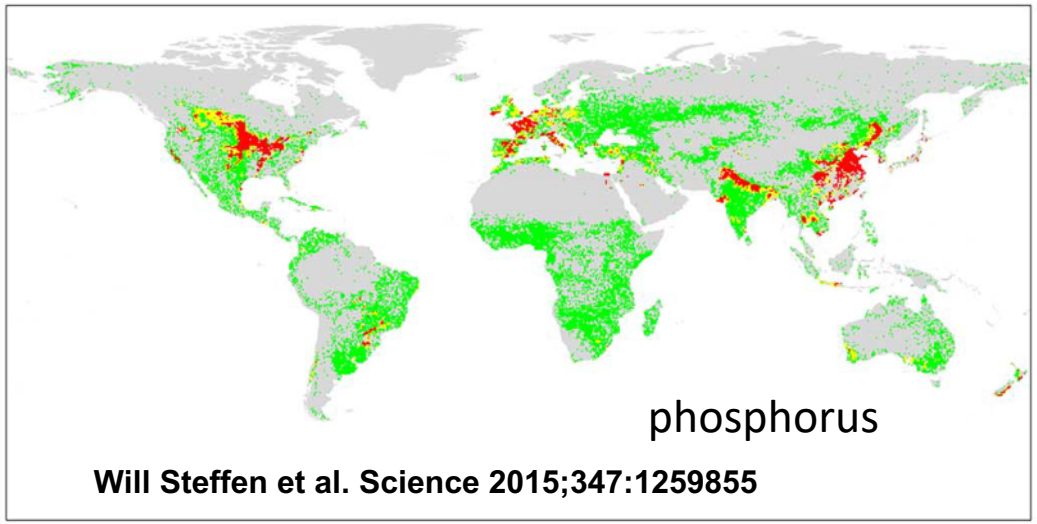



- Watersheds protect the Nation's water supply by
  - Buffering precipitation inputs
  - Filtering sediments
  - Biogeochemically transforming contaminants and excess nutrients
- Watershed function is stressed by global change
  - Increases in contaminant and nutrient inputs
  - Changing precipitation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

IDEAS Watersheds

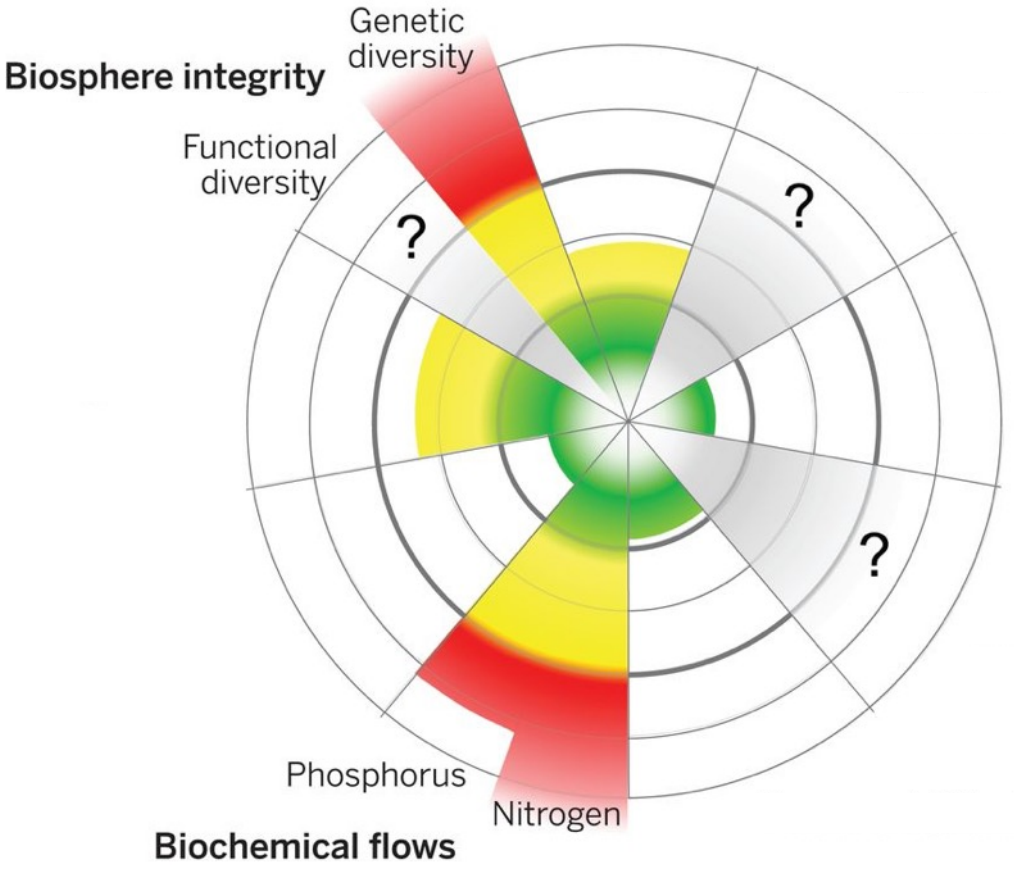
# Biogeochemical Flows Have Reached a Critical Global Threshold

- Nutrient inputs have surpassed the processing capacity of the global terrestrial system
- Thousands of impaired waters in the US
- Sensitive to climate and land use change




Will Steffen et al. Science 2015;347:1259855

Rockstrom et al.'s Planetary Boundaries

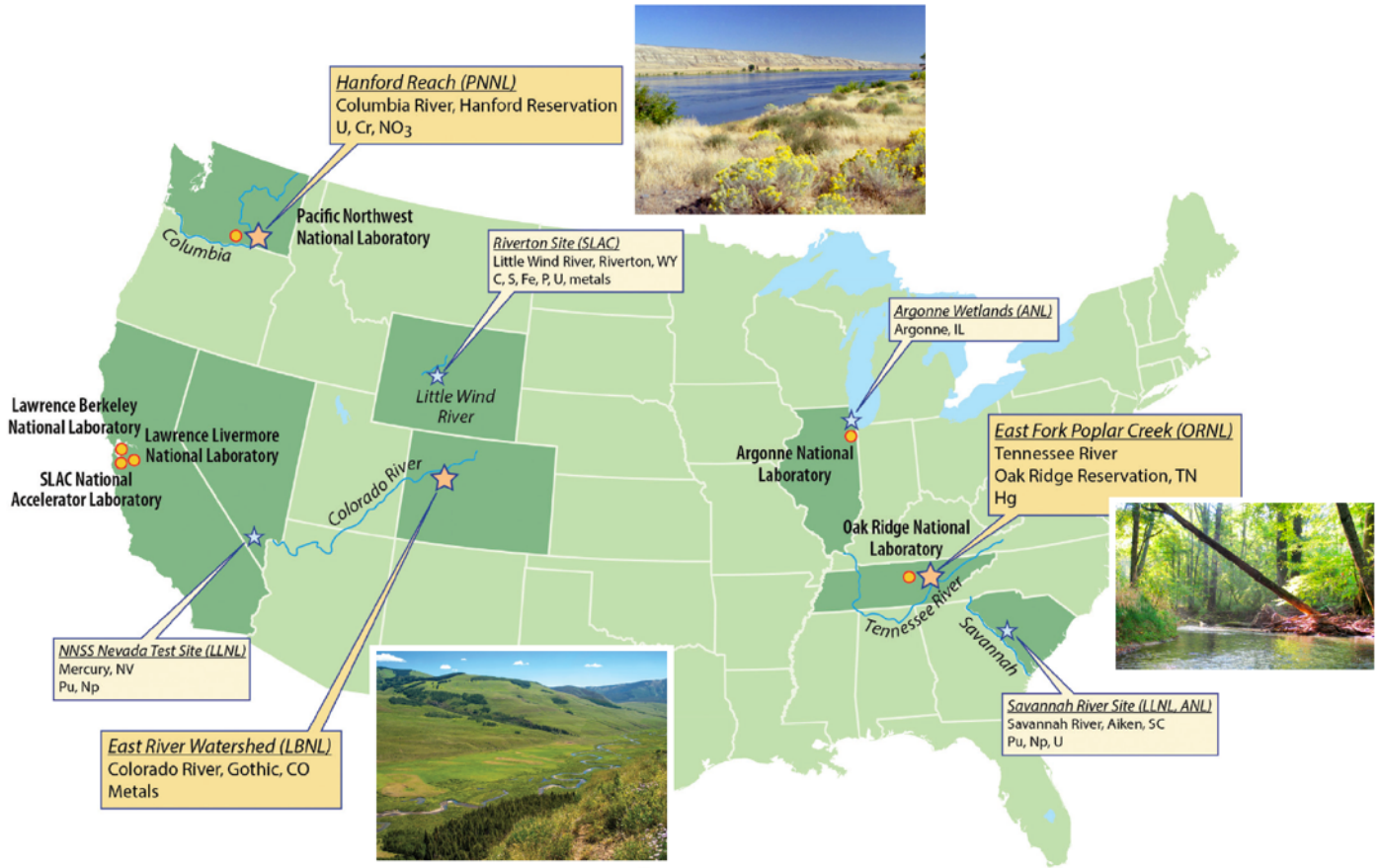



Will Steffen et al. Science 2015;347:1259855

IDEAS Watersheds

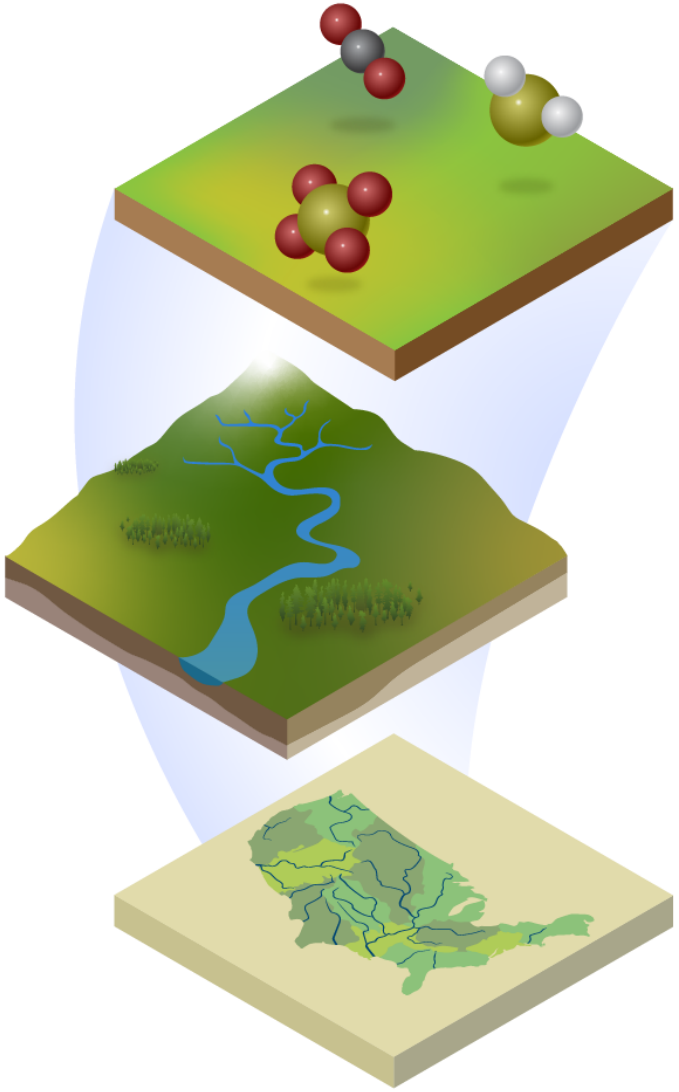
# SBR Seeks a Robust Predictive Understanding of Watershed Hydrobiogeochemical Function

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




IDEAS Watersheds

# Three Cornerstones of SBR Watershed Science



## 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

## 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

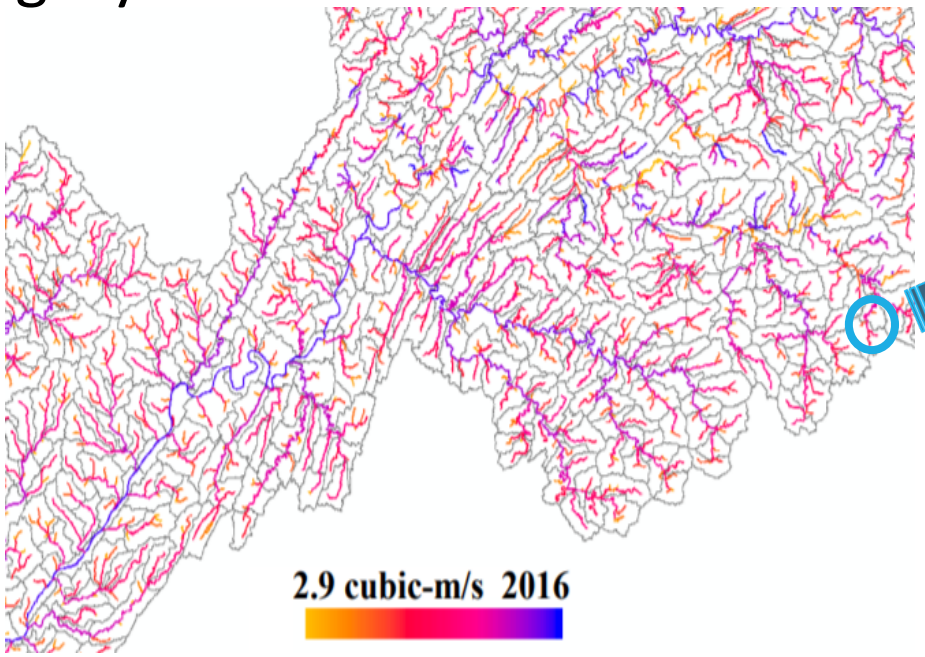


*Support SBR development of a robust predictive understanding of watershed hydrobiogeochemical function.*

IDEAS Watersheds

# Challenges in Computational Watershed Science

- Integration across scales – tractably representing detailed process understanding at societally relevant scales
- Managing process complexity
- Changing and uncertain computer architectures
- Existing capability is fragmented and in legacy codes



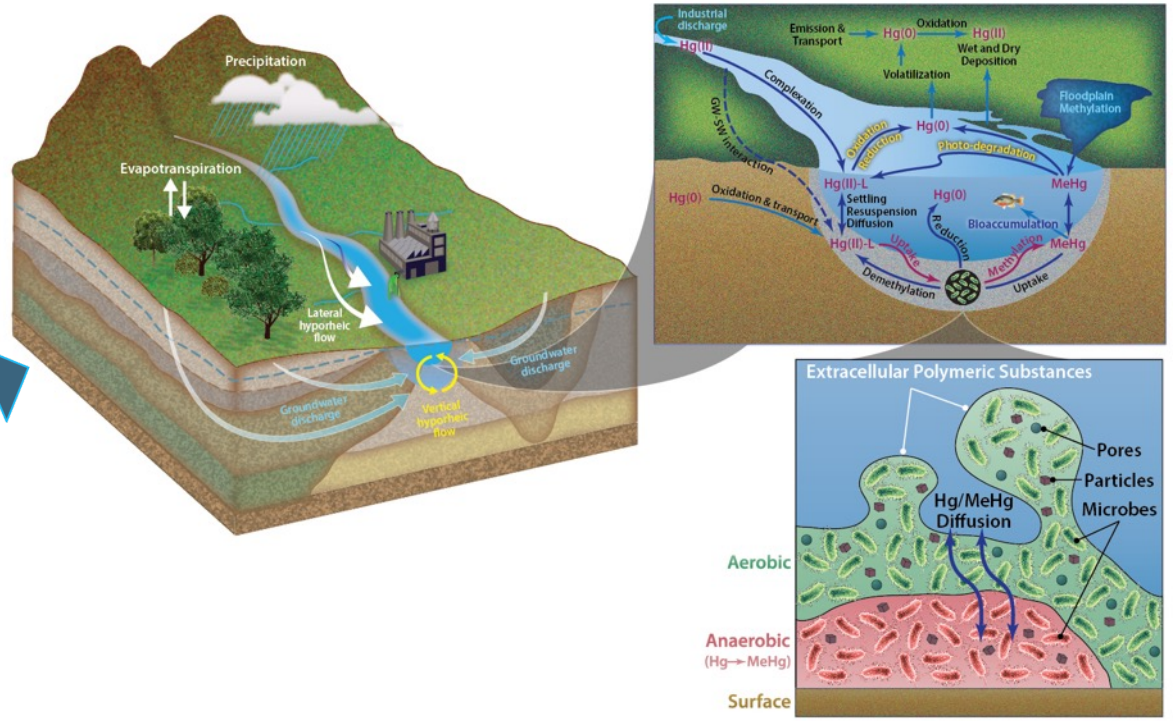
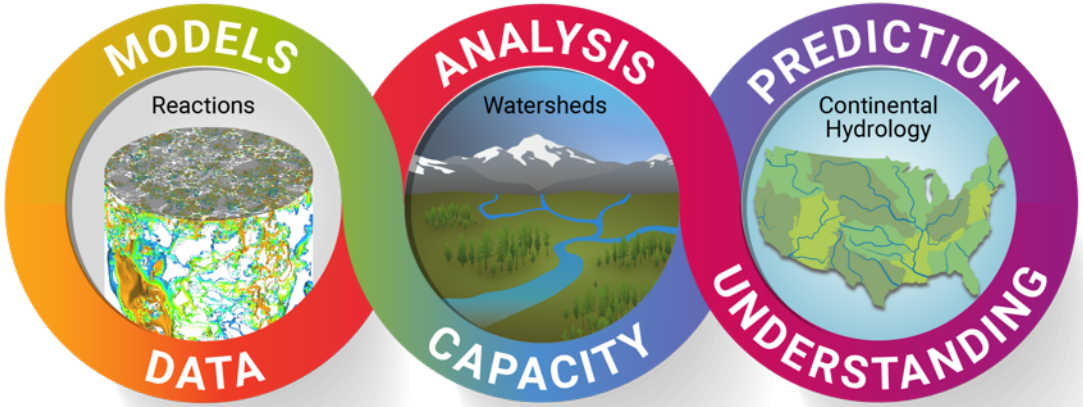




Image credit: Sujith Nair, ORNL

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).

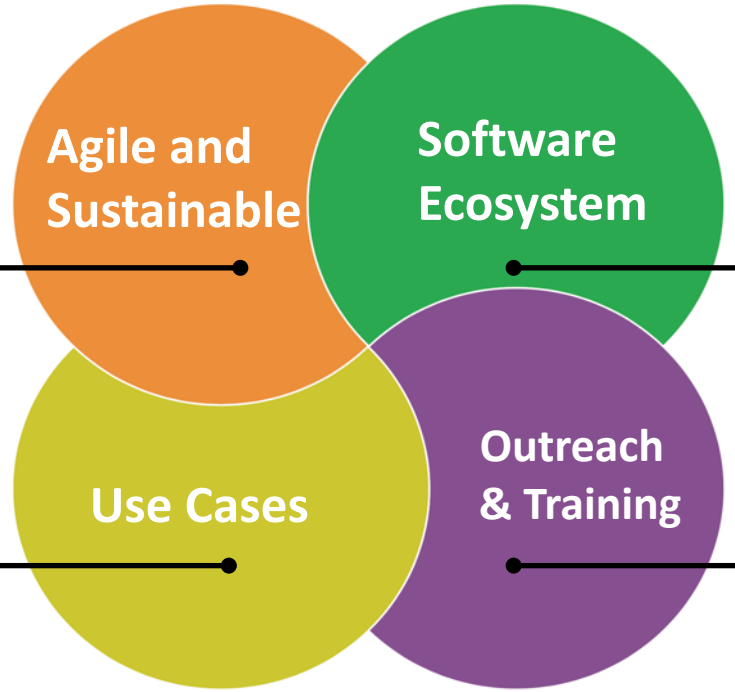
***APPROACH***

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.**

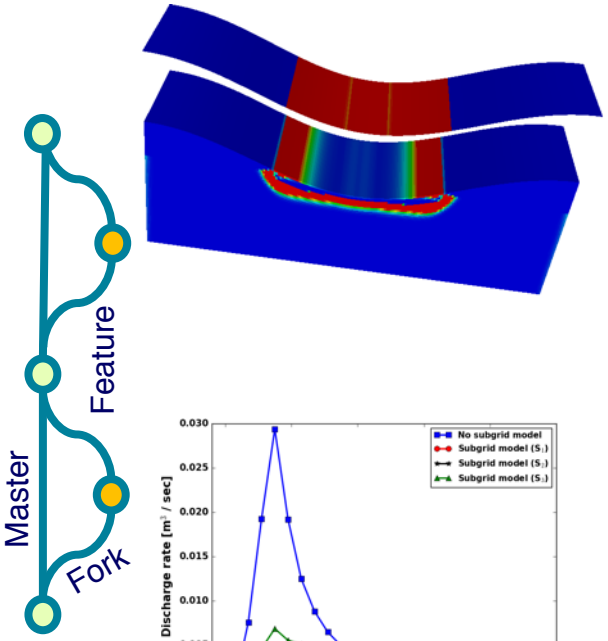


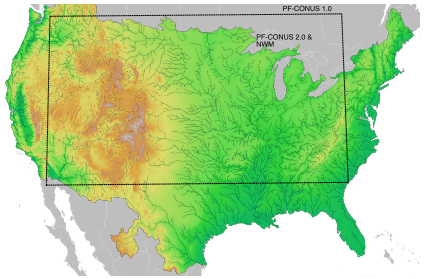



IDEAS Watersheds

# IDEAS-Watersheds Builds on IDEAS Phase 1

- Interoperability and the Software Ecosystem
  - Developed an integrated hydrology reactive transport capability using an interoperable approach (ATS-Amanzi+Alquimia+PFLOTRAN).
- Methodologies
  - Explored roles of ***software maintainers***, and embedded computational science developers.
- Multiscale Modeling Framework in DOE Next-Generation Ecosystem Experiments (NGEE-Arctic) Project
  - Developed and published subgrid model for microtopography effects on overland flow
  - Delivered intermediate-scale model using this new framework
- CONUS
  - Developed new 250m and 1km model domains (including coastline) that align with the National Water Model (NWM) grid
  - Intercompared simulation output between ParFlow and NWM and a suite of observations



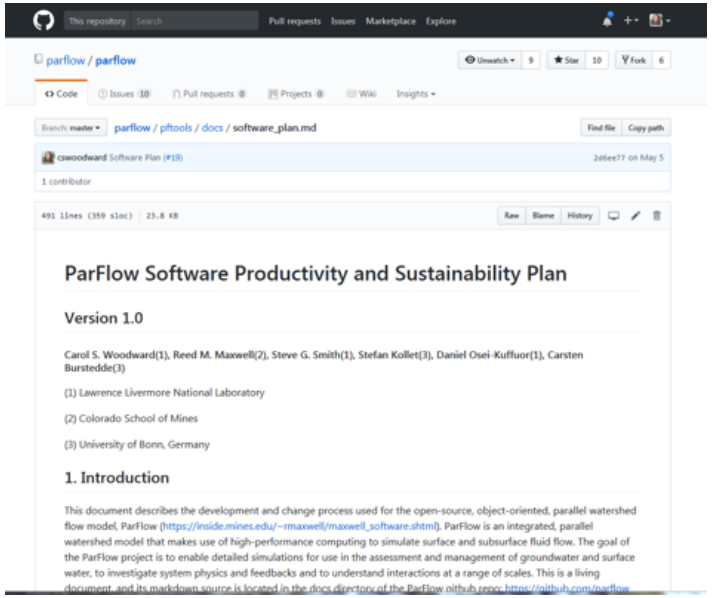



IDEAS Watersheds

# Codes need Maintainers

## Ensures sustainability for community developed software

- Software design
  - Review design documents and proposals for new features
  - Ensure maintainability and extensibility
- Software repository and workflows
  - Support code reviews
  - Provide new releases, archiving old releases.
- Ensure documentation is added for new features
- Maintain software configuration and build system
- Manage testing and continuous integration



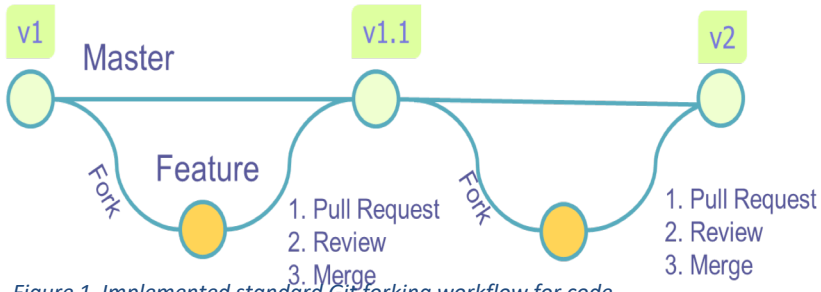



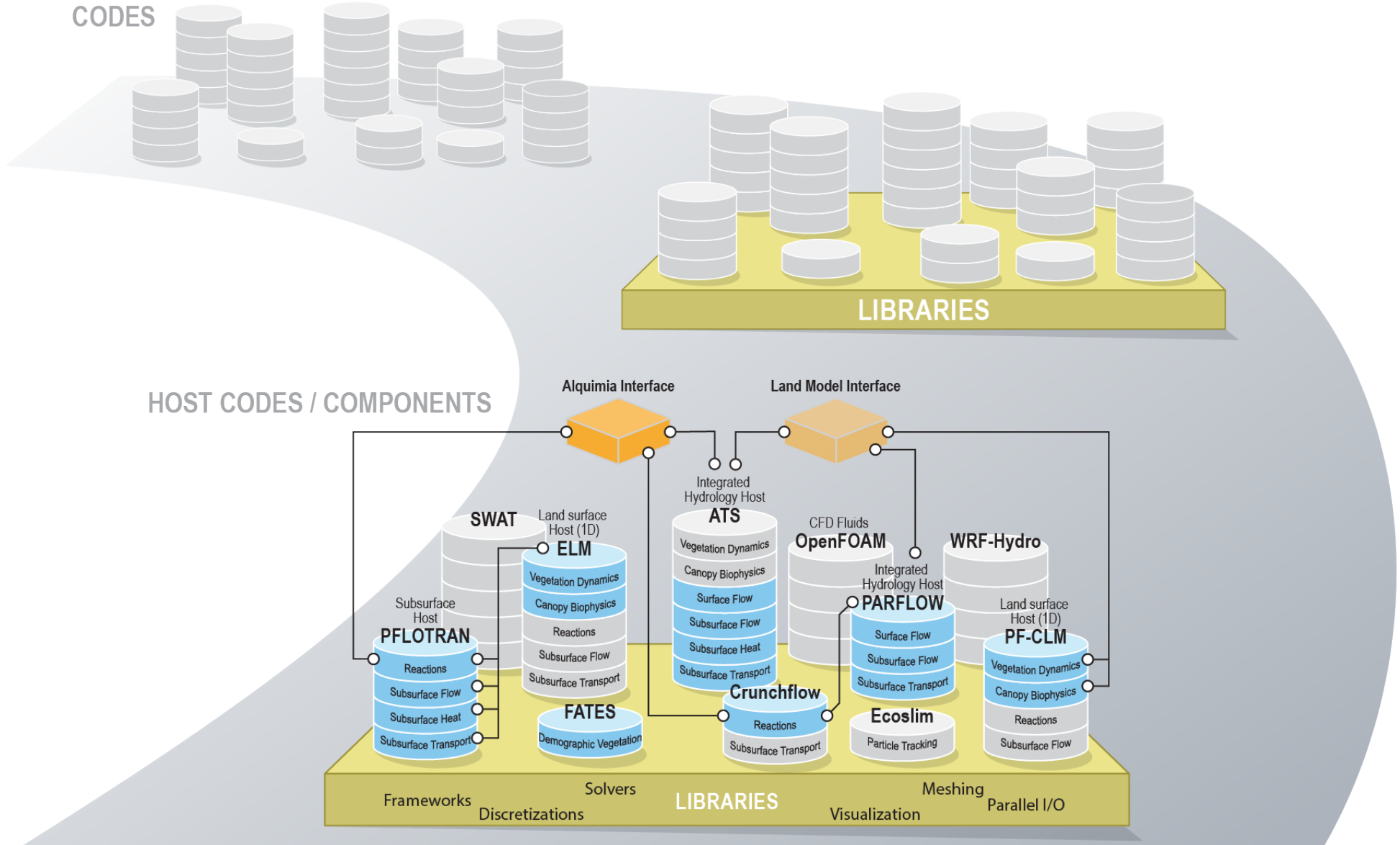

*Figure 1 Implemented standard Git forking workflow for code development in the ParFlow GitHub repository.*

*Demonstrated the importance of Maintainers with the ParFlow code/community in our CONUS work.*

IDEAS Watersheds

# IDEAS-Watersheds Software Ecosystem

## From Silos to an Ecosystem

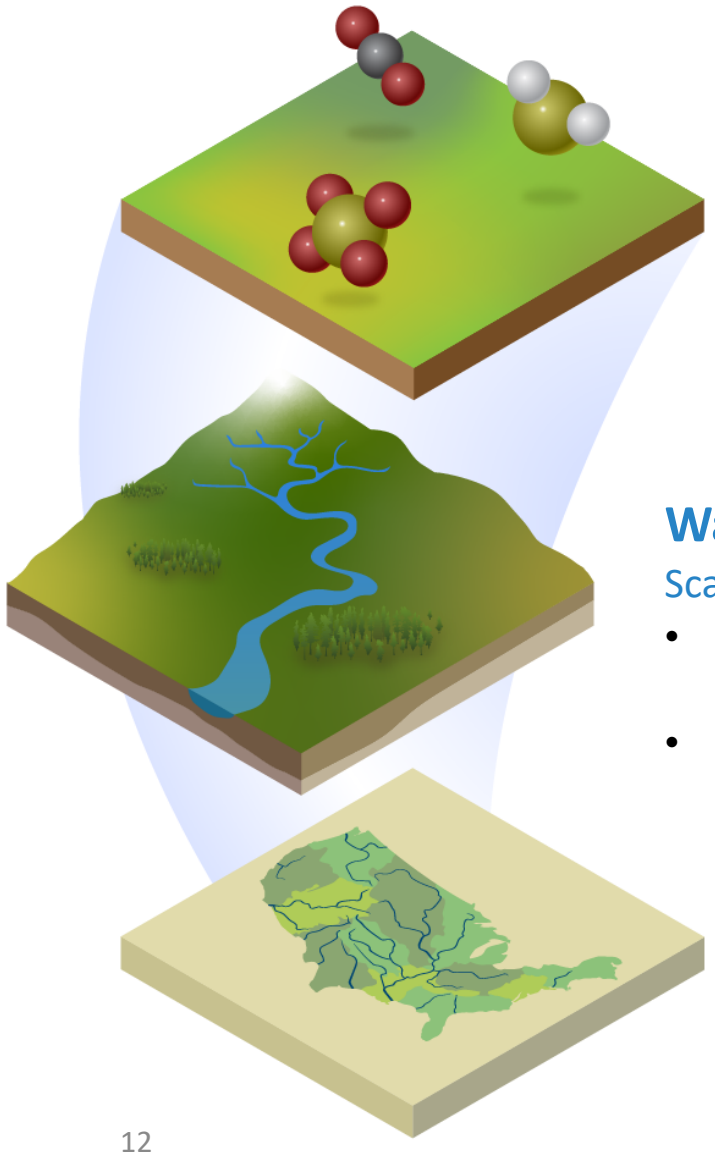



xSDK

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

IDEAS Watersheds

# IDEAS-Watersheds Research 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

## Watershed hydrobiogeochemistry

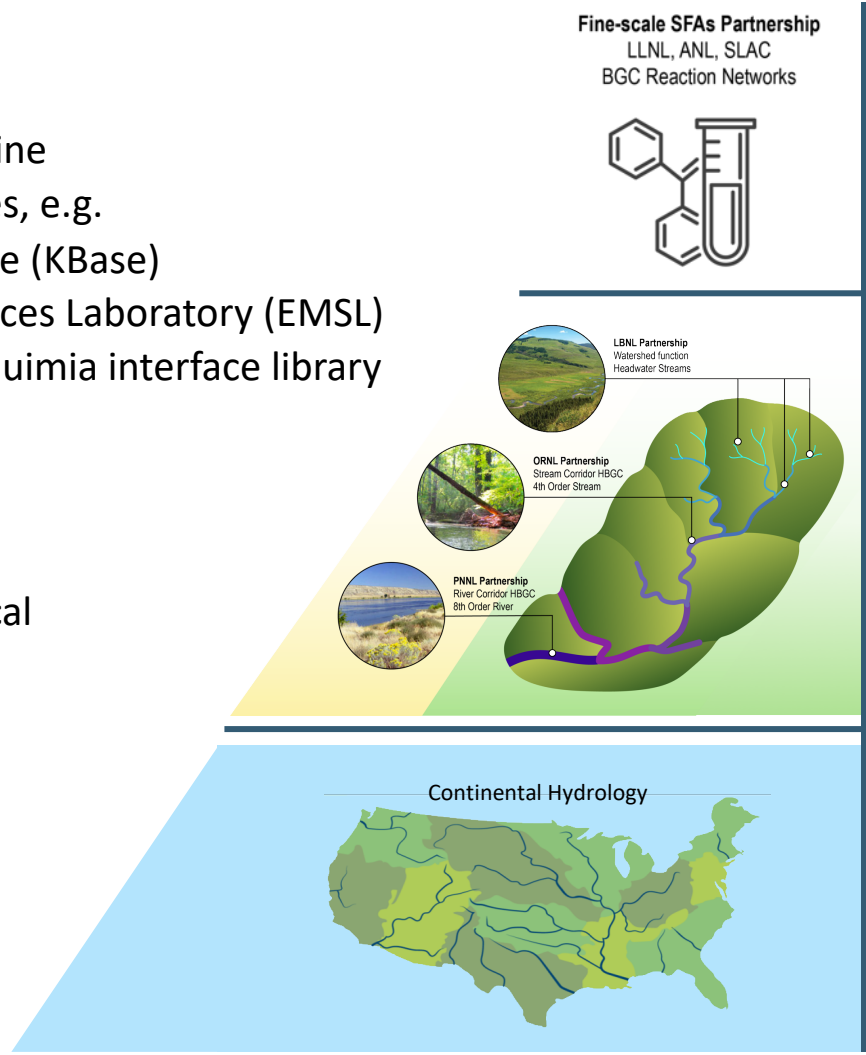
### Scaling to watersheds

- 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

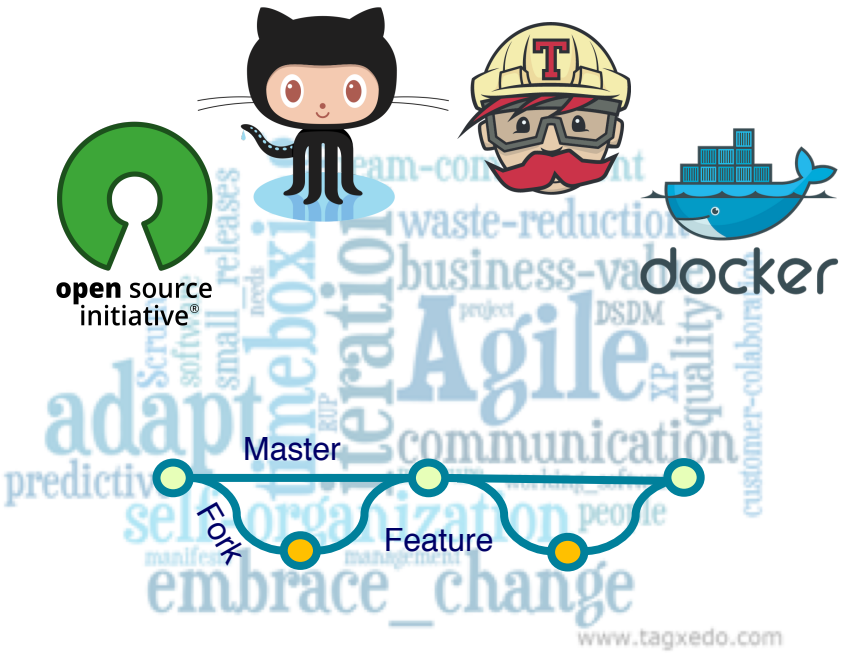


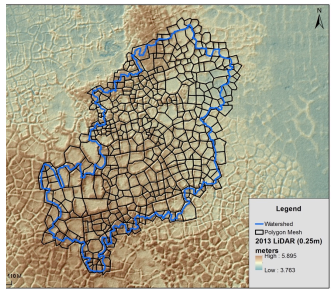

IDEAS-Watersheds Shared Infrastructure

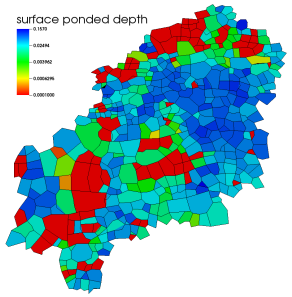


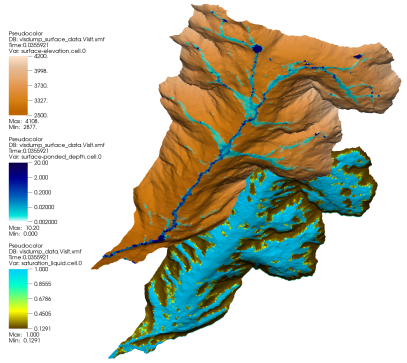
IDEAS Watersheds

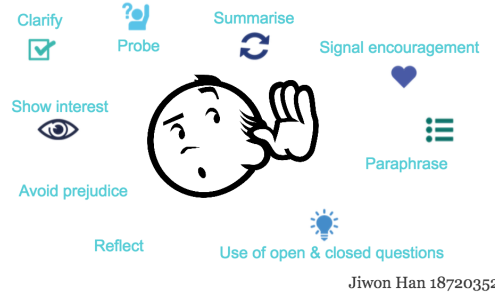
# Agile + Use Cases + Design Thinking





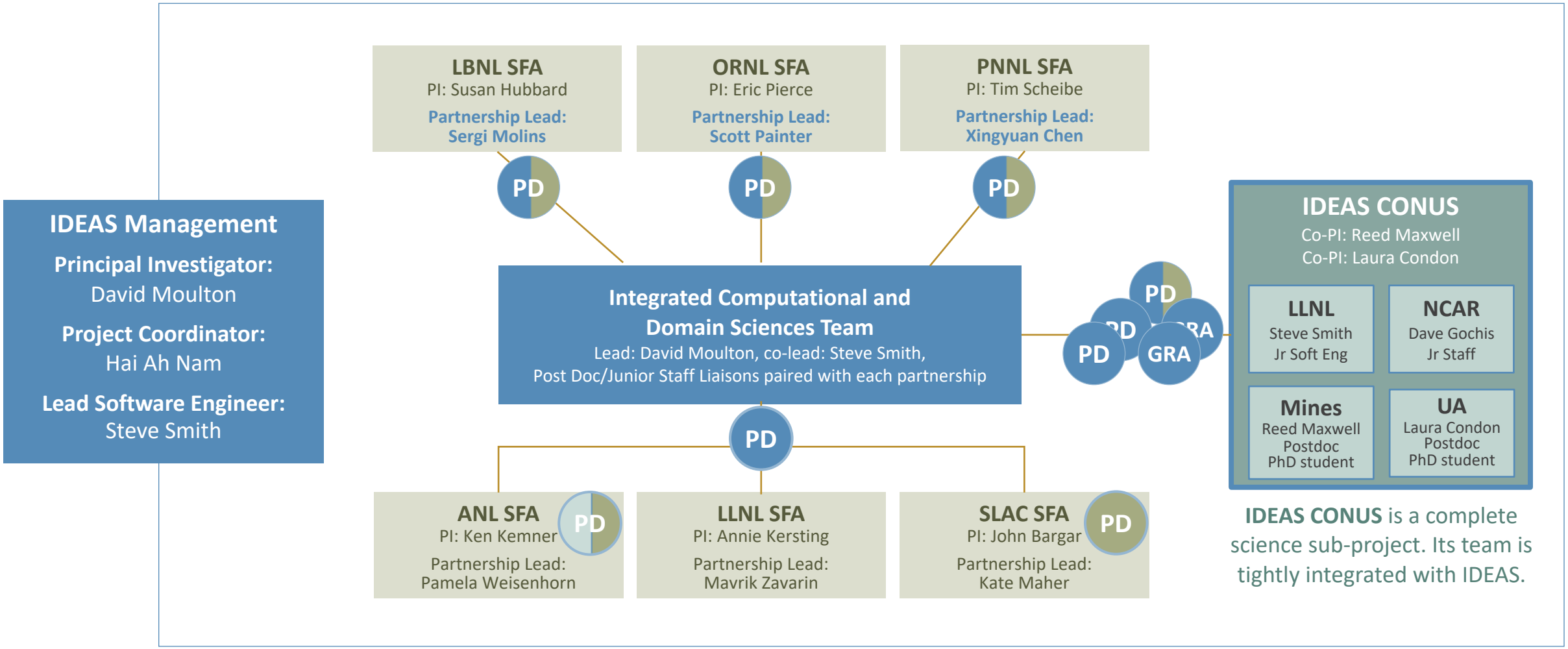

Tools and Methodologies ensure developer productivity of open, sustainable, flexible, and portable software ecosystem.

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

Design Thinking: Adds empathy and active listening to problem framing and ideation.

IDEAS Watersheds

# IDEAS-Watersheds: Integration and Training




**IDEAS CONUS** is a complete science sub-project. Its team is tightly integrated with IDEAS.

IDEAS Watersheds

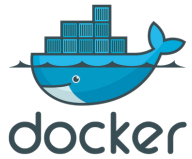
# Sustainable Software Ecosystem
## Requires the people and culture to make it flourish

- Integrated Computational and Domain Sciences team
  - Interdisciplinary
    - Computational science
    - Earth science
  - Led by PI and Senior Software Engineer
  - Composed of jointly funded postdocs and junior staff
- The team will
  - Receive training in modern agile development methodologies and workflows
  - Engage in virtual sprints for specific development tasks
  - Participate in outreach activities such as contributing to the Better Scientific Software (BSSw.io) blogs
  - Participate in high-performance computing training & webinars
- Once trained, this pool will be used to provide host code maintainers

IDEAS Watersheds

# Sustainable Software Ecosystem
## Requires everyone embrace best practices

- Open development as much as open source
  - Public git repository, including feature development
  - Branches, pull requests …
- Documentation and community outreach
  - Design document and Developers guide
  - User Guides, tutorials, short courses
- Easy Deployment
  - Robust portable build system, and containers
- Continuous Integration
  - Automated testing with excellent coverage
- Continuous Improvement
  - Process for evaluation and improvement (e.g., IDEAS-ECP PSIP)

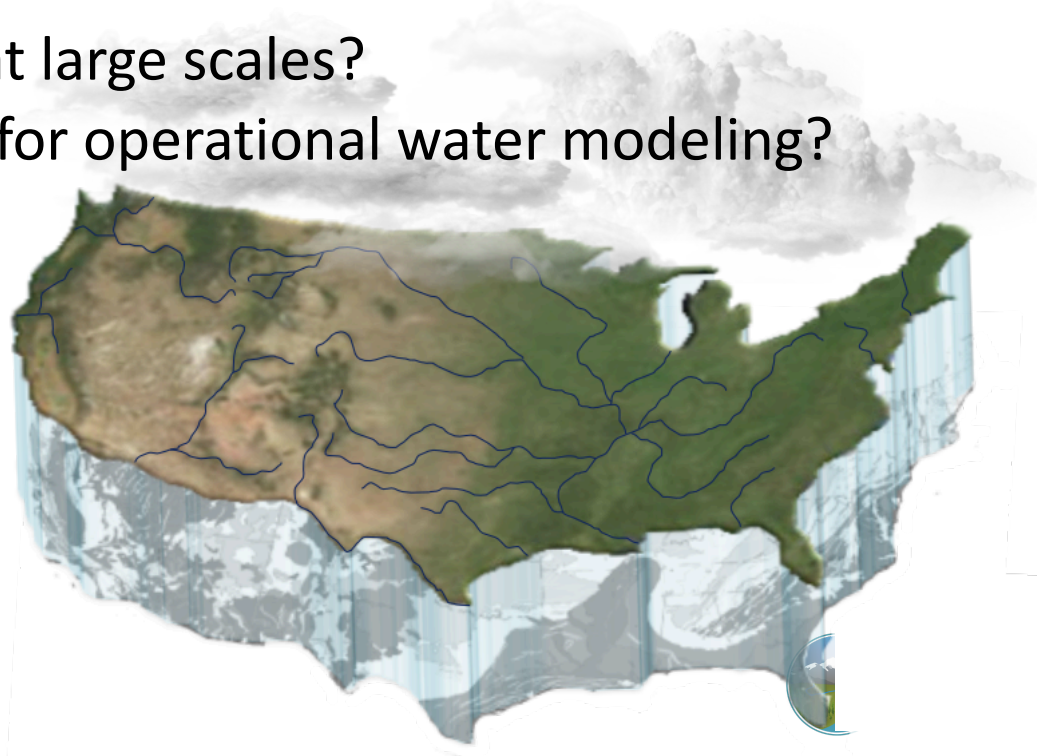



# IDEAS-Watersheds CONUS

## Bridging scales and understanding processes with integrated hydrologic simulations

- **Science questions:**
  - What is the role of lateral groundwater flow and hydrologic exchanges across spatial scales?
  - At what spatial scales and physical settings does lateral groundwater flow have the largest impact on watershed behavior?
  - How do flow paths and residence times vary at large scales?
  - What is the correct groundwater formulation for operational water modeling?

- **Science challenge:** Developing hyper-resolution continental scale hydrologic models that capture three dimensional variably saturated flow



# Critical Cultural Challenge:

## Software and Papers need equal recognition

nature COMMUNICATIONS

ARTICLE

https://doi.org/10.1038/s41467-020-14688-0 OPEN

Check for updates

### Evapotranspiration depletes groundwater under warming over the contiguous United States

Laura E. Condon [1✉], Adam L. Atchley [2] & Reed M. Maxwell [3]

A warmer climate increases evaporative demand. However, response to warming depends on water availability. Existing earth system models represent soil moisture but simplify groundwater connections, a primary control on soil moisture. Here we apply an integrated surface-groundwater hydrologic model to evaluate the sensitivity of shallow groundwater to warming across the majority of the US. We show that as warming shifts the balance between water supply and demand, shallow groundwater storage can buffer plant water stress; but only where shallow groundwater connections are present, and not indefinitely. As warming persists, storage can be depleted and connections lost. Similarly, in the arid western US warming does not result in significant groundwater changes because this area is already largely water limited. The direct response of shallow groundwater storage to warming demonstrates the strong and early effect that low to moderate warming may have on groundwater storage and evapotranspiration.

https://uanews.arizona.edu/story/groundwater-depletes-arid-american-west-moving-east

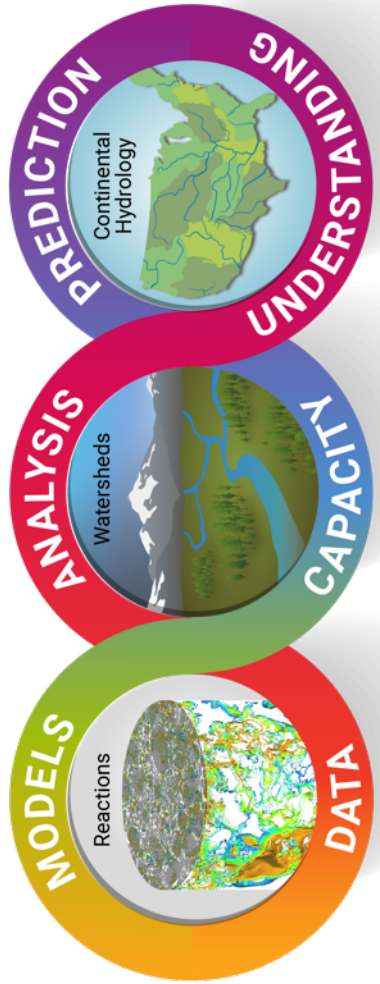
Our sponsors appreciate the challenge, but still value papers more.

IDEAS Watersheds

# IDEAS-Watersheds

## Integrate and broaden the impact of the SBR cornerstones and testbeds

- Enhance productivity in watershed science.
- Create a more viable and sustainable 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 junior computational scientists geared toward interdisciplinary teams and adaptable sustainable software.






IDEAS Watersheds

# Q&A