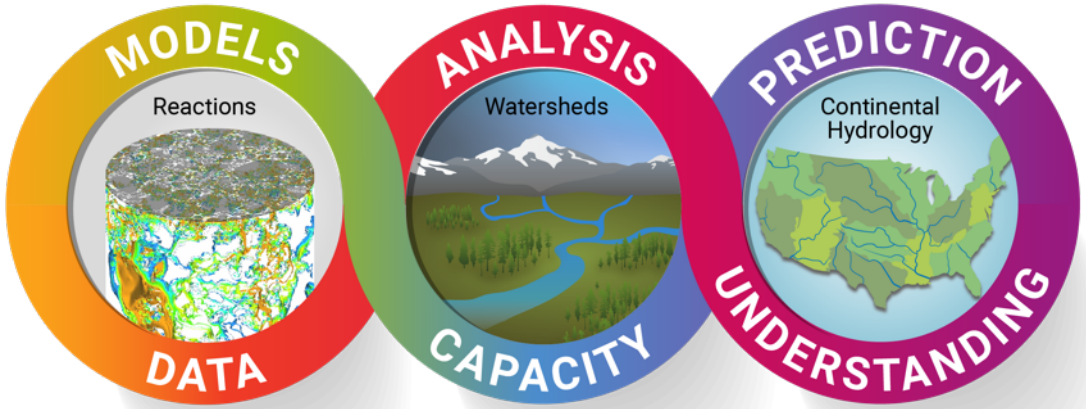
IDEAS-Watersheds

Accelerating watershed science through a community-driven software ecosystem



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)

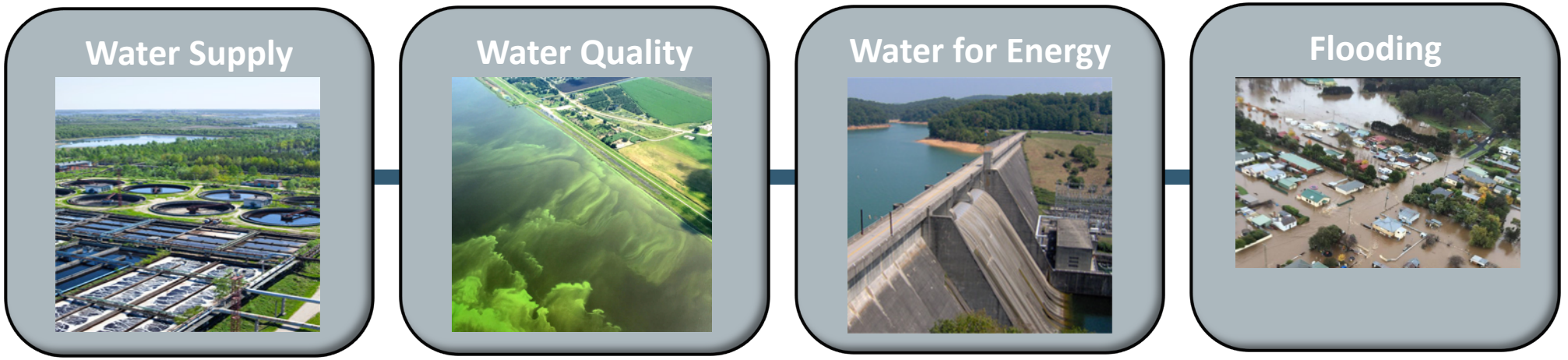
U.S. DEPARTMENT OF ENERGY | Office of Science

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

LA-UR-20-28193

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

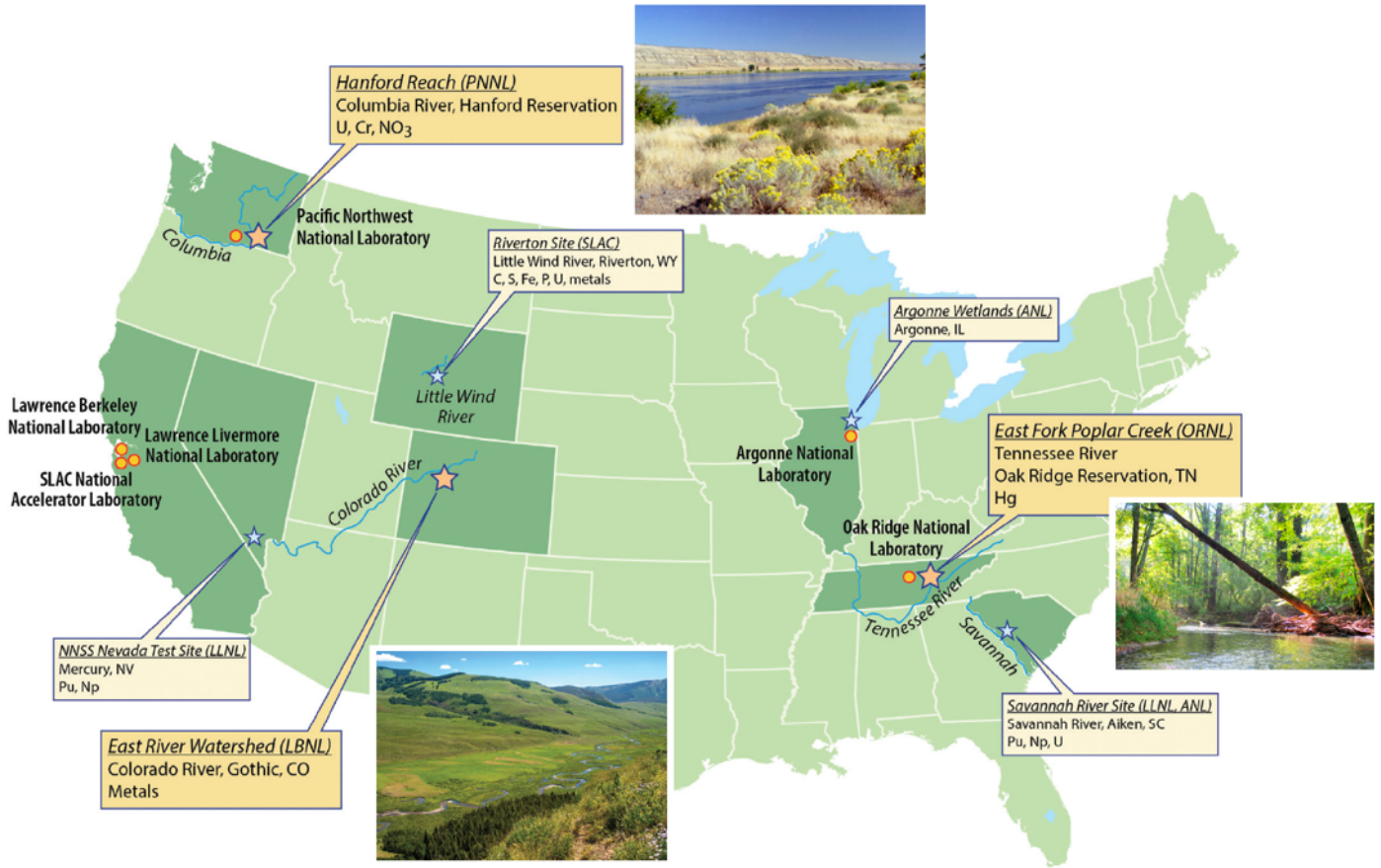


- Watersheds protect the Nation's water supply by
  - Buffering precipitation inputs
  - Filtering sediments
  - Biogeochemically transforming contaminants and excess nutrients
- Watershed function is stressed by global change
  - Increases in contaminant and nutrient inputs
  - Changing precipitation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

IDEAS WATERSHEDS

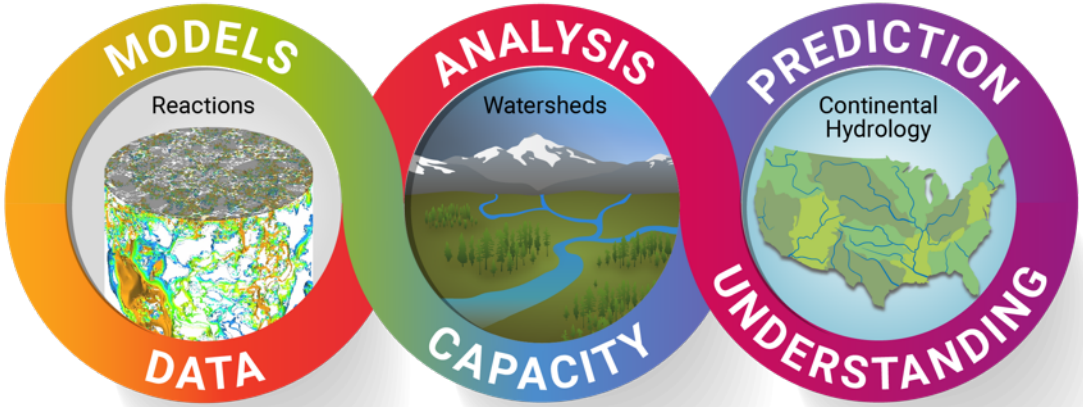
SBR Seeks a Robust Predictive Understanding of Watershed Hydrobiogeochemical Function

- 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

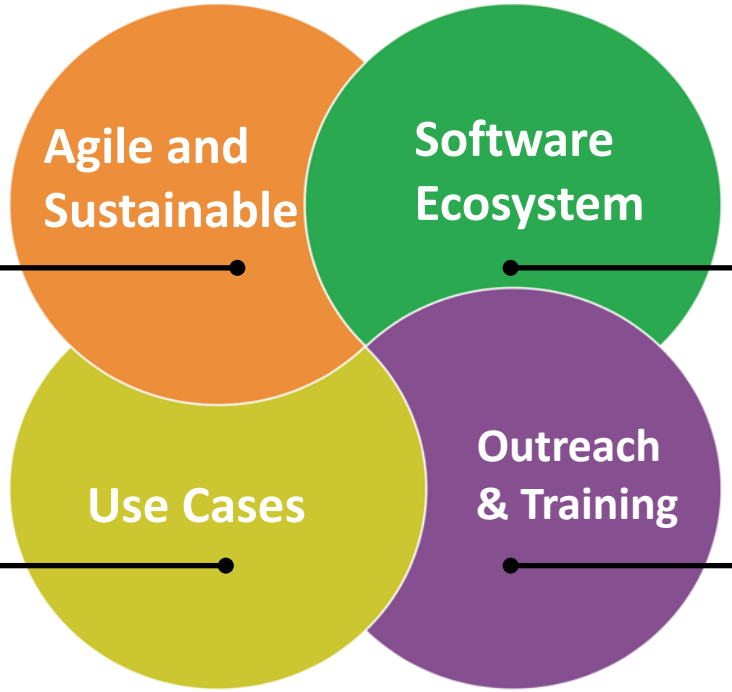
Increase scientific productivity by improving software, advancing community shared capabilities, and realizing the potential of advanced computing resources.

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

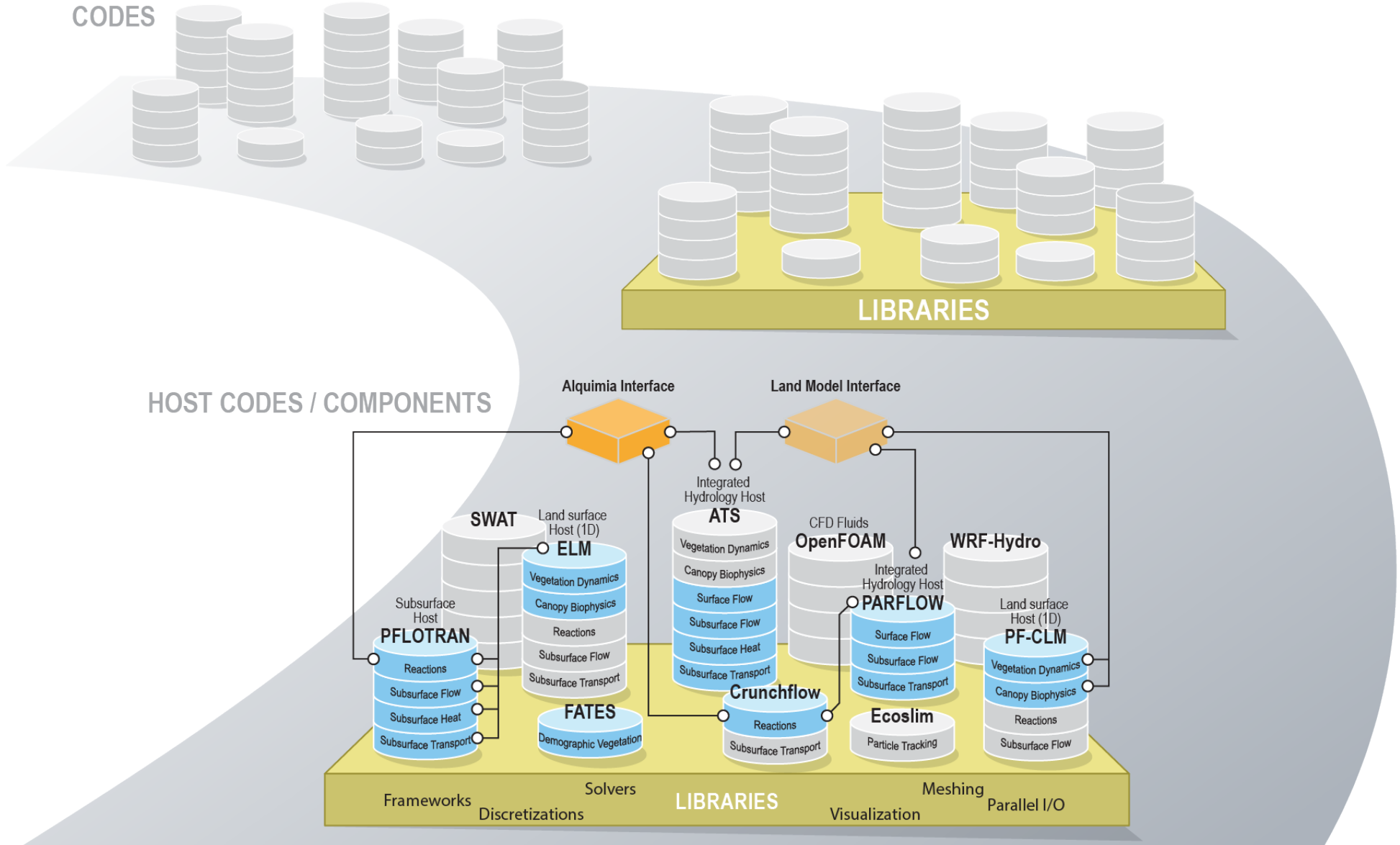
Create **partnerships** between IDEAS and SFAs centered on concrete Use Cases with shared deliverables.

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

IDEAS WATERSHEDS

IDEAS-Watersheds Software Ecosystem

From Silos to an Ecosystem

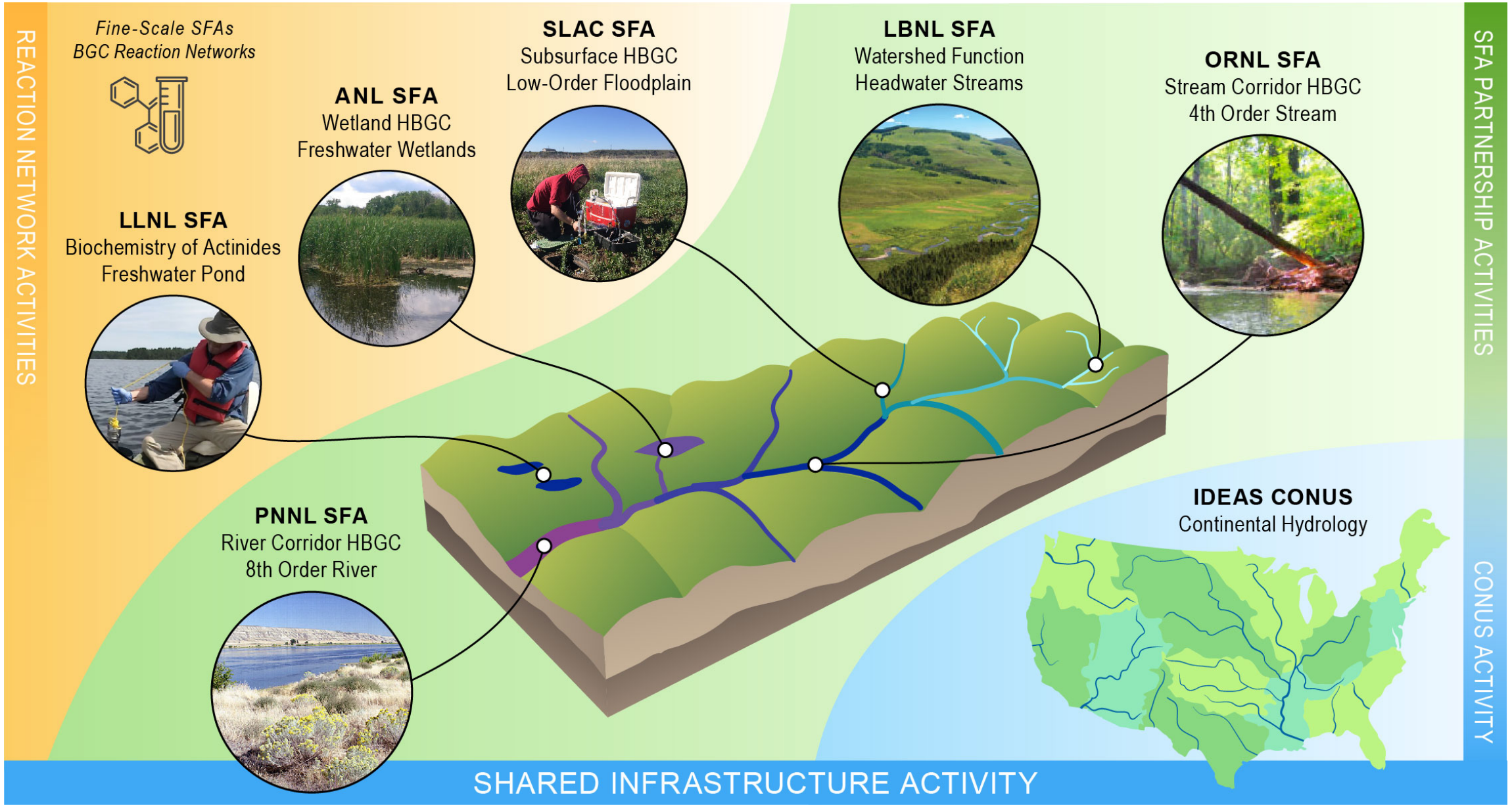


xSDK

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

IDEAS WATERSHEDS

IDEAS-Watersheds Research Activities



IDEAS-Watersheds: Integration

IDEAS Management

Principal Investigator:
David Moulton

Project Coordinator:
Hai Ah Nam

Lead Software Engineer:
Steve Smith

Hai Nam

Steve Smith

LBNL SFA
PI: Susan Hubbard
Partnership Lead: Sergi Molins

ORNL SFA
PI: Eric Pierce
Partnership Lead: Scott Painter

PNNL SFA
PI: Tim Scheibe
Partnership Lead: Xingyuan Chen

PD PD PD

Integrated Computational and Domain Sciences Team
Lead: David Moulton, co-lead: Steve Smith,
Post Doc/Junior Staff Liaisons paired with each partnership

PD PD GRA PD GRA

PD

ANL SFA PD
PI: Ken Kemner
Partnership Lead: Pamela Weisenhorn

LLNL SFA
PI: Annie Kersting
Partnership Lead: Mavrik Zavarin

SLAC SFA PD
PI: John Bargar
Partnership Lead: Kate Maher

IDEAS CONUS
Co-PI: Reed Maxwell
Co-PI: Laura Condon

LLNL
Steve Smith
Jr Soft Eng

NCAR
Dave Gochis
Jr Staff

Mines
Reed Maxwell
Postdoc
PhD student

UA
Laura Condon
Postdoc
PhD student

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

Integrated Computational and Domain Sciences (Distributed) Team is key to training junior staff in software engineering and modeling, and integration through bi-weekly meetings on

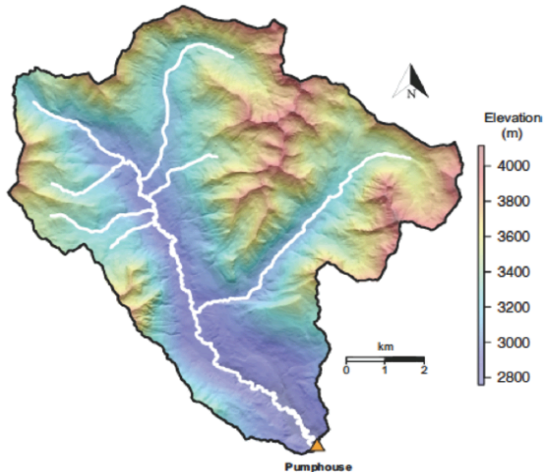
IDEAS WATERSHEDS

Partnership with Watershed Function SFA (LBNL)

Workflows to generate multi-resolution meshes for multiphysics simulations in mountainous watersheds

Lead: Sergi Molins

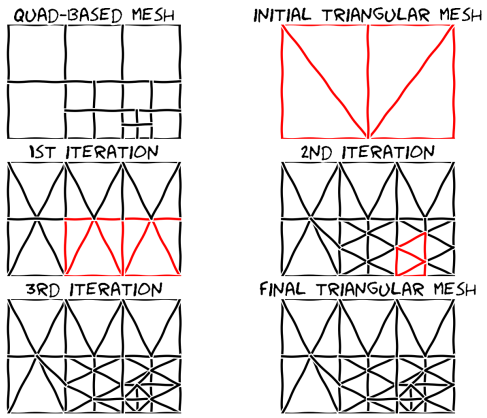
Hubbard et al (2018) VZJ

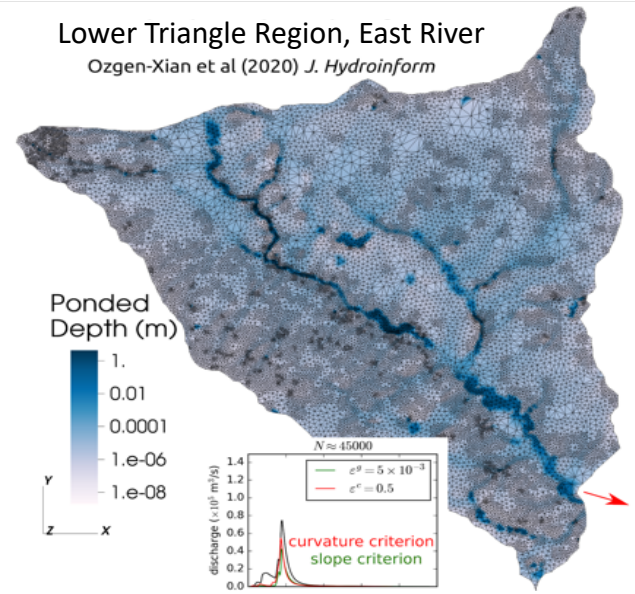


East River, CO
Digital Elevation Map (DEM)

- Pronounced gradients in hydrology, geomorphology, vegetation, and weather
- Perturbations in watershed dynamics at seasonal to decadal timescales

- Wavelet-based refinement criterion from rectangular data to unstructured mesh
- General approach allows for single-parameter refinement criteria



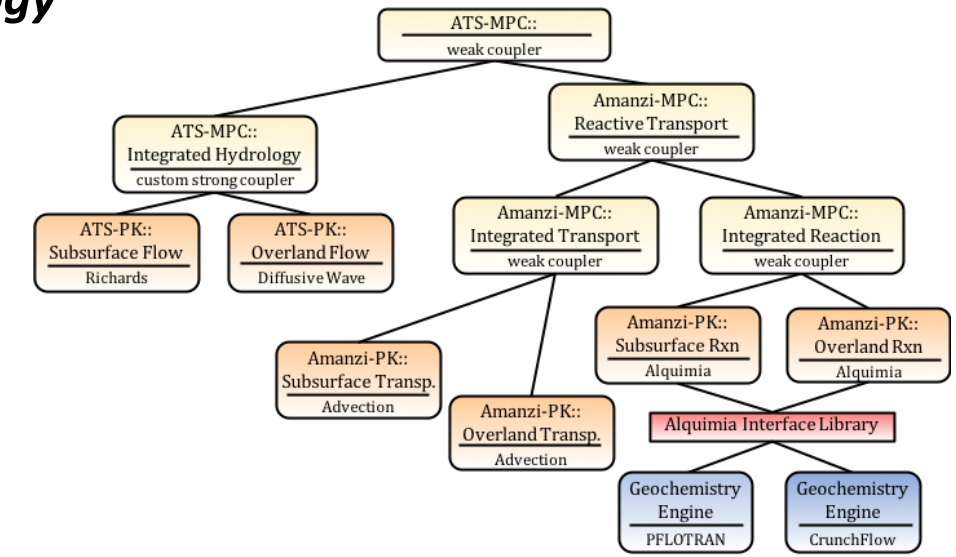


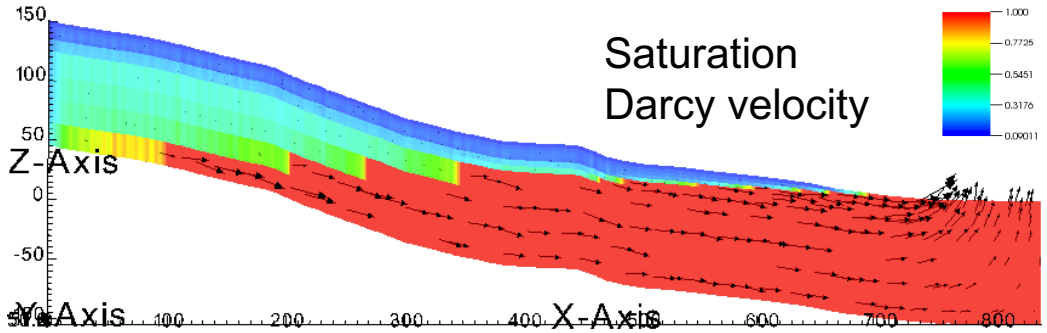
IDEAS WATERSHEDS

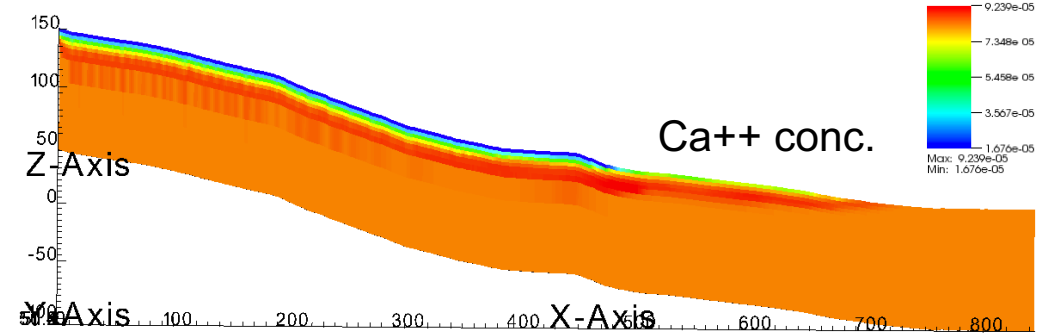
Partnership with Watershed Function SFA (LBNL)

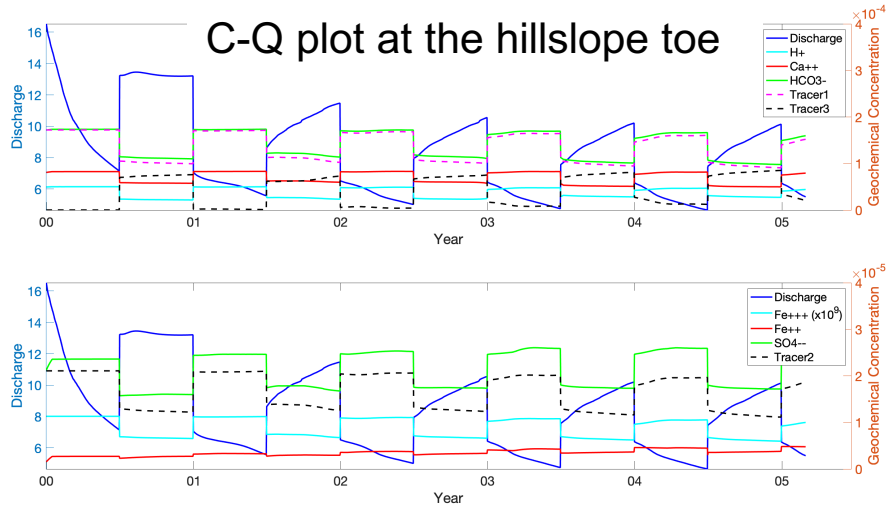
Surface/Subsurface Reactive Transport for Integrated Hydrology

- ATS using PFlotran and CrunchFlow via Alquimia
- Hillslope simulations with dynamic forcing
- Reaction network focused on pyrite and calcite dissolution dynamics associated with water table evolution
- Effluent concentrations and solid phase evolution









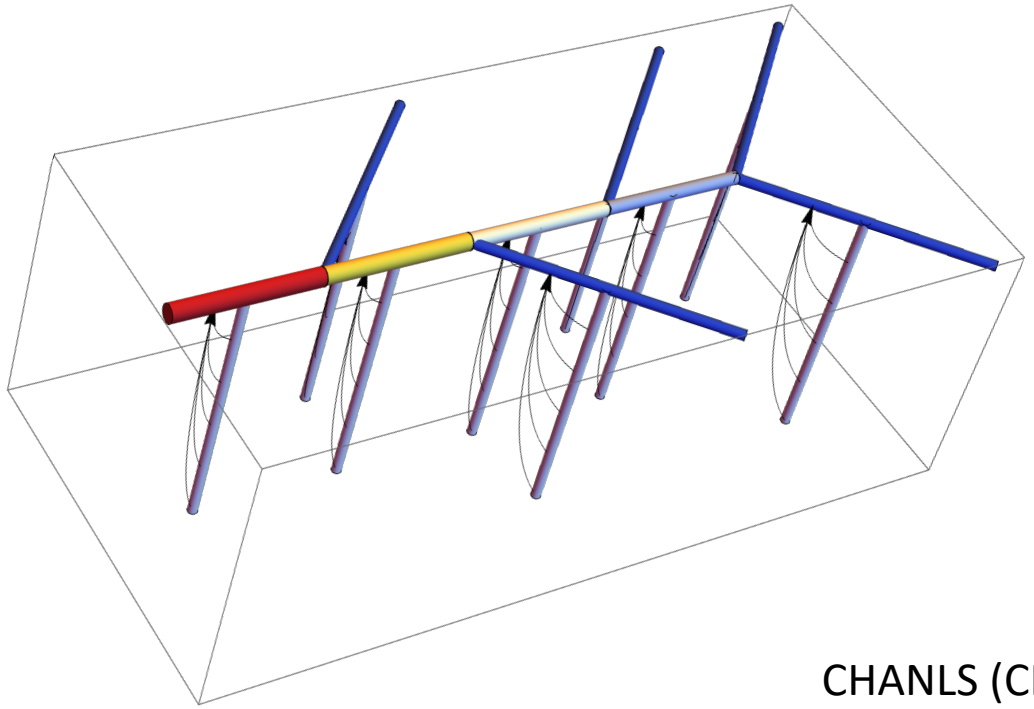
Z. Xu et al (in progress)

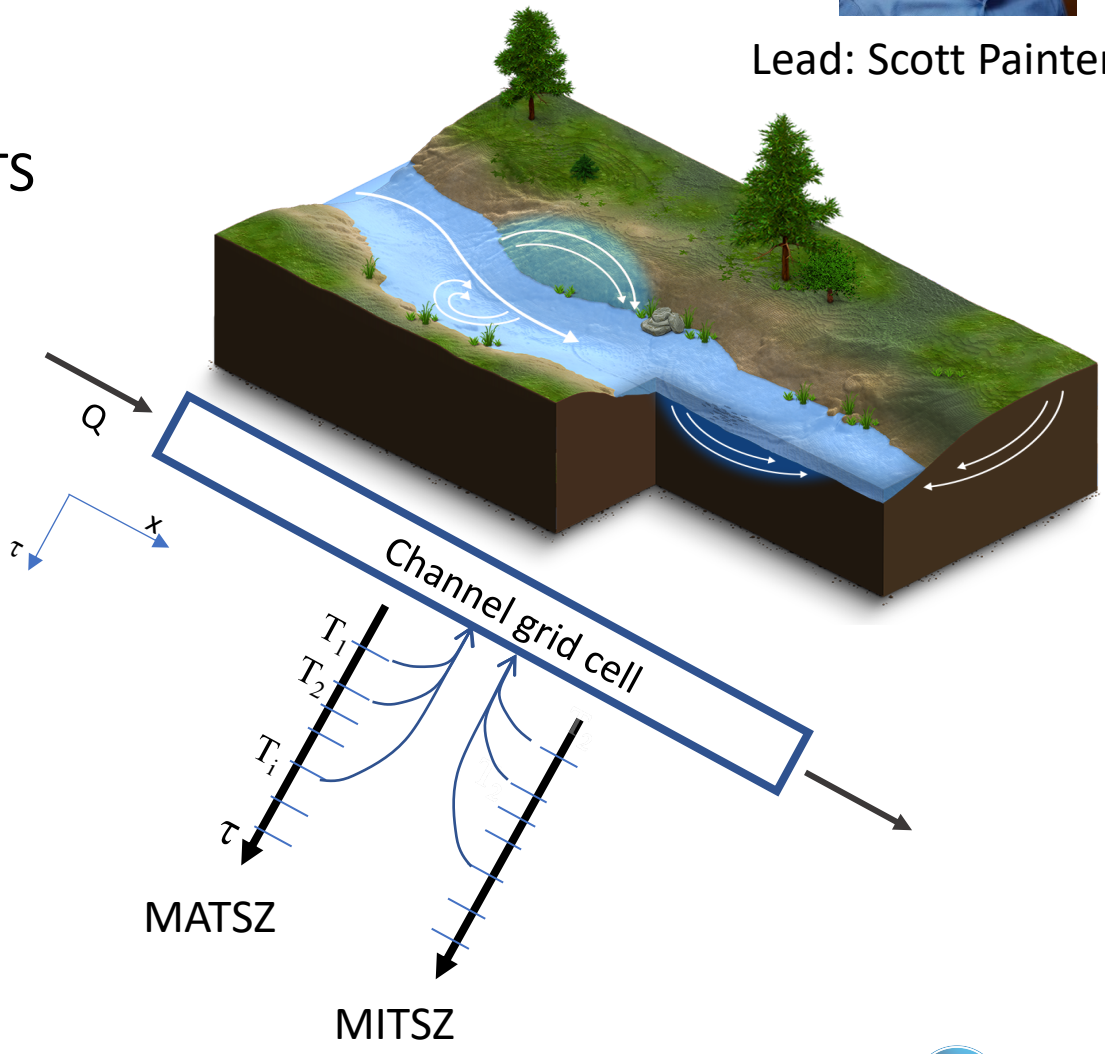
Partnership with Critical Interfaces SFA (ORNL)

Lead: Scott Painter

ATS implementation of multiscale CHANLS model (Painter 2018) for reactive transport in fluvial corridors

- Leverages flexible multiphysics framework in ATS
- Accounts for effects of metabolically active transient storage zones (MATSZs)
- Remains tractable at basin scales



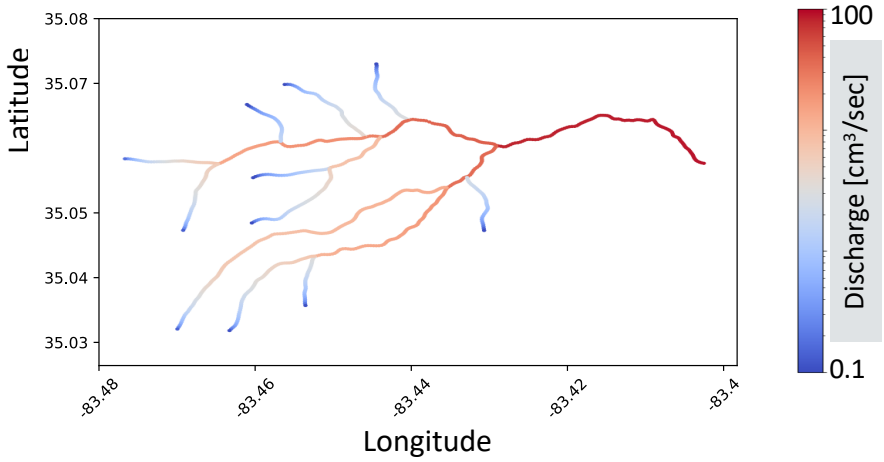


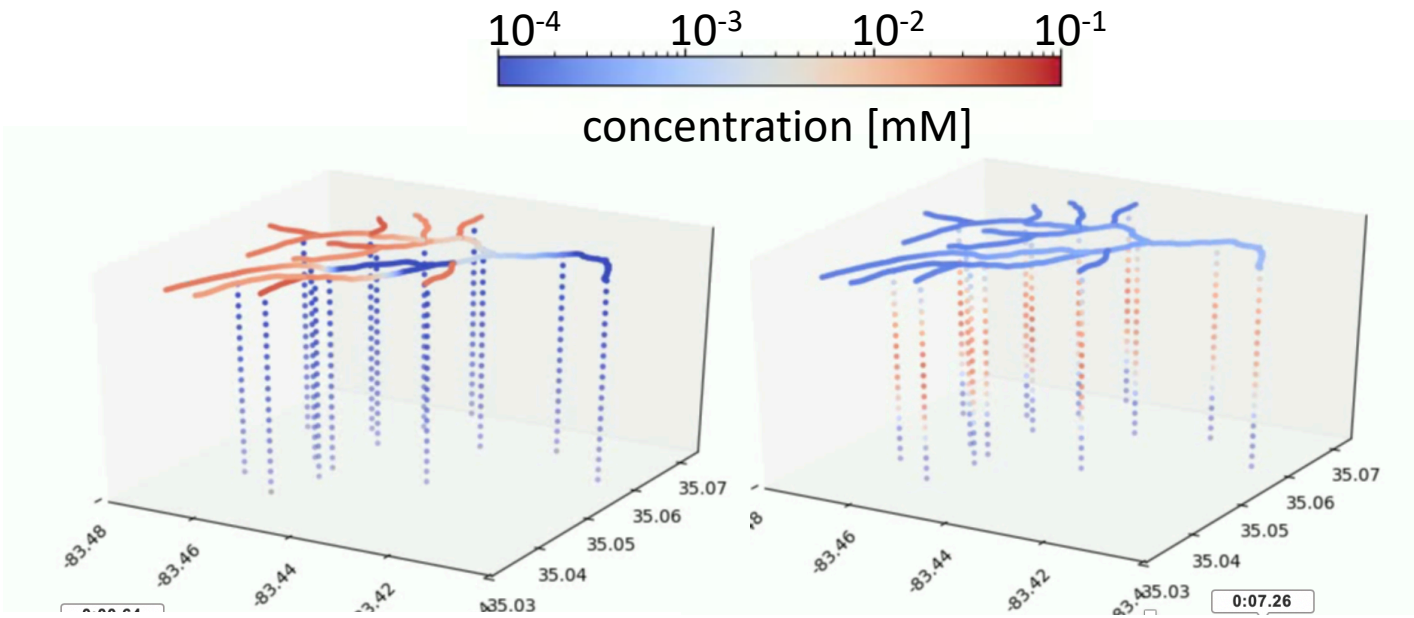
CHANLS (CHAnel Network with Lagrangian Subgrid) model

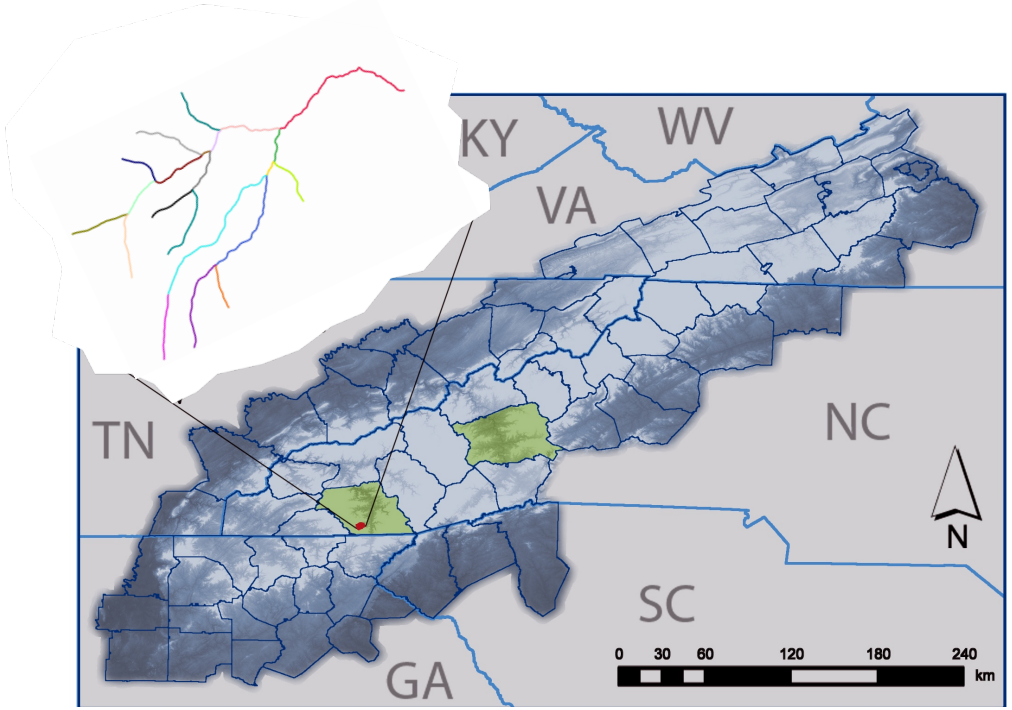
IDEAS WATERSHEDS

Partnership with Critical Interfaces SFA (ORNL)

- Watershed-scale implementation in ATS with reactions from PFLOTRAN
  - Automated construction of stream channel network from online data sources (NHDplus)
  - Attach hyporheic subgrid mesh to each channel grid cell
  - Alquimia interface extended to work with subgrid mesh
  - Benchmarking in progress

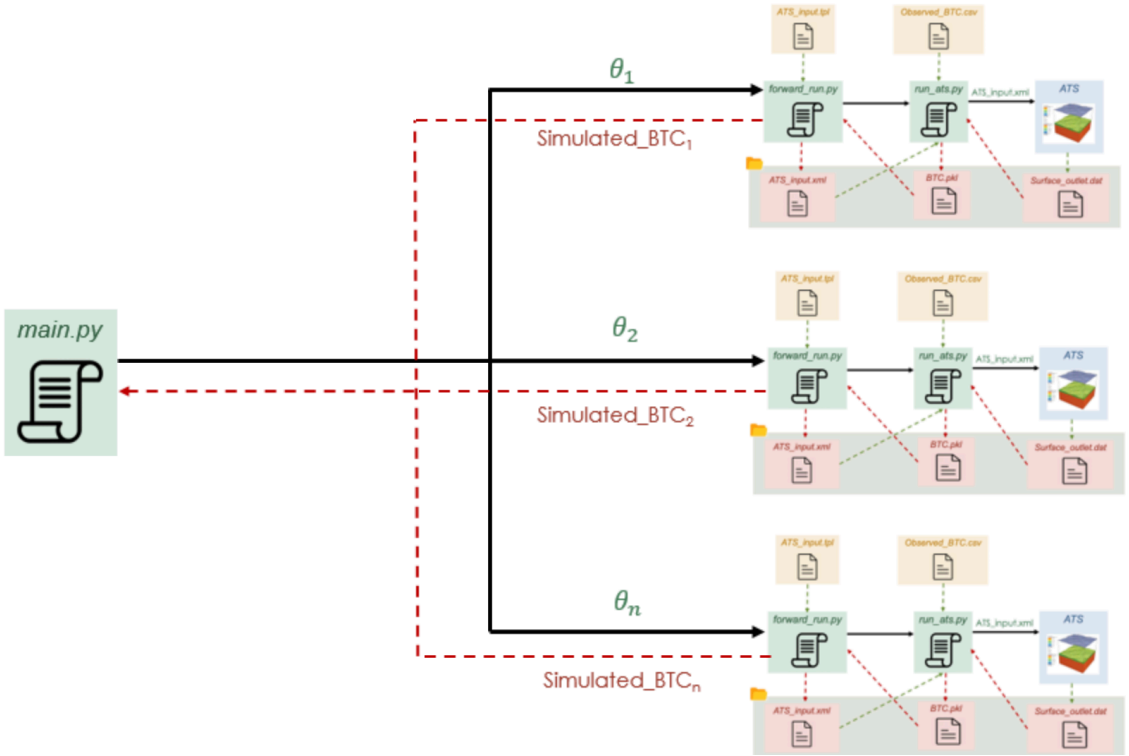


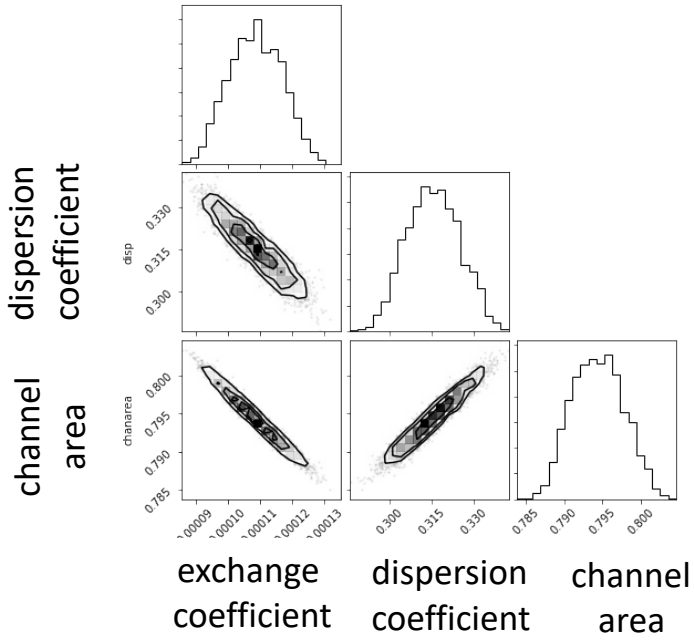


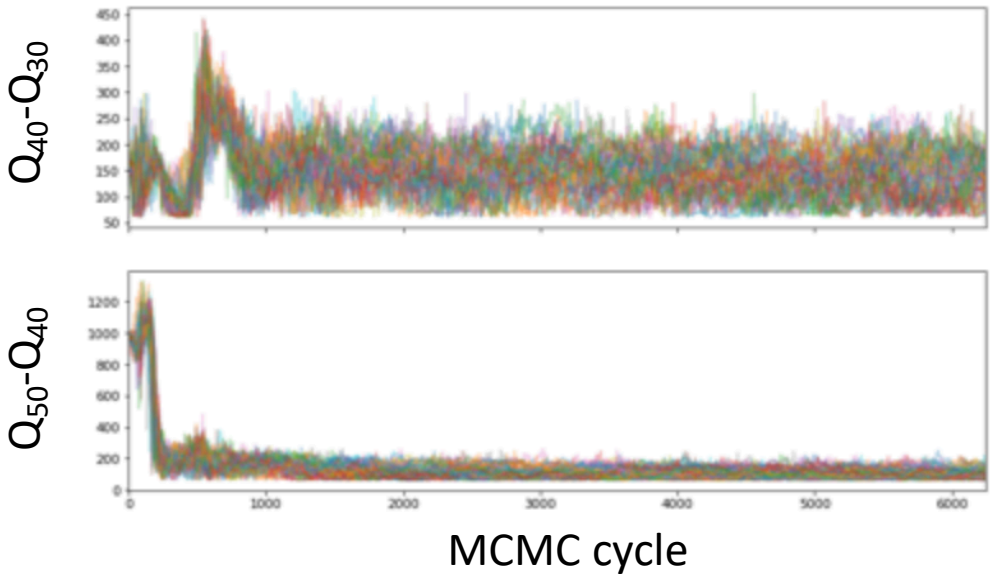


Partnership with Critical Interfaces SFA (ORNL)

- Jupyter notebook workflows for parameter estimation from tracer test results
  - Optimization
  - Markov Chain Monte Carlo for UQ
  - Multicore capability (parallel chains)
  - Non-parametric representation of hyporheic lifetime distribution

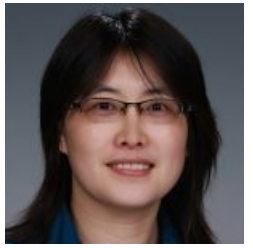






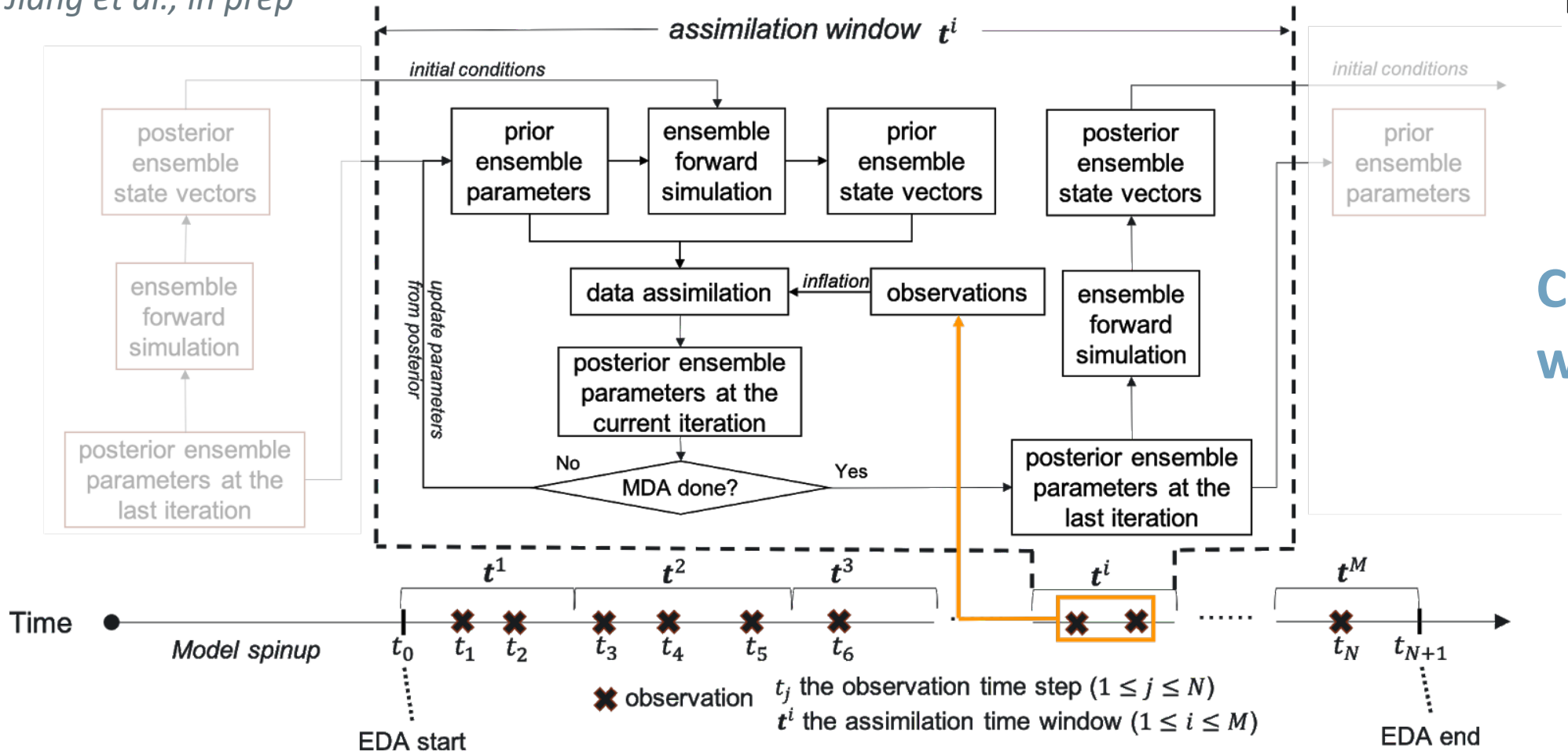
Partnership with River Corridor SFA (PNNL)

Developed Data Assimilation Capability for Flow and Reactive Transport: DART-PFLOTRAN



Lead: Xingyuan Chen

Jiang et al., in prep



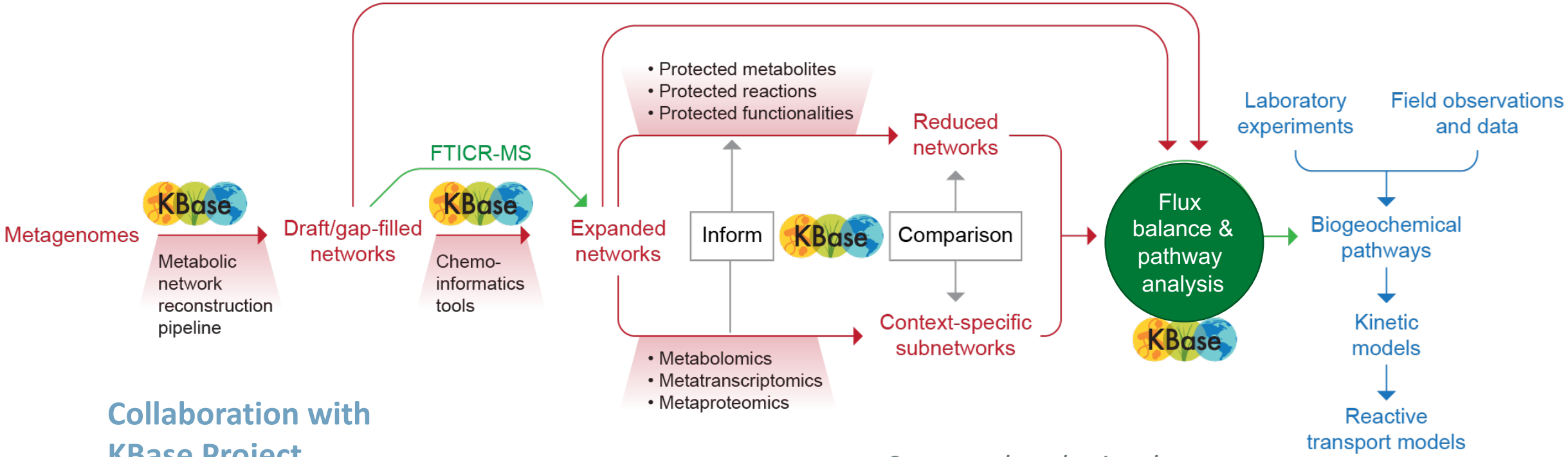
Collaboration with NCAR

DART: Data Assimilation Research Testbed

IDEAS WATERSHEDS

Partnership with River Corridor SFA (PNNL)

Leveraging KBase Pipeline to Inform Reactive Transport Modeling



Collaboration with KBase Project

Song et al., submitted

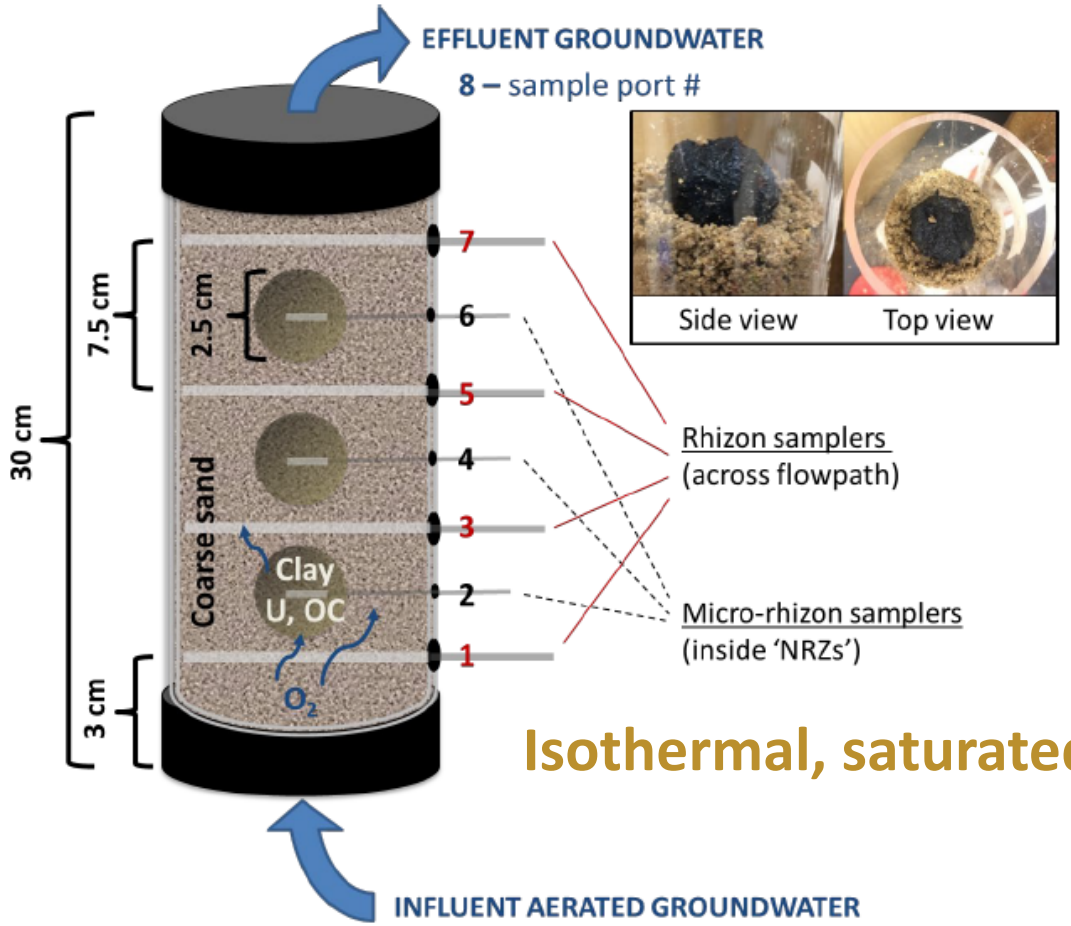
PFLOTRAN

ThermoStoichWizard:

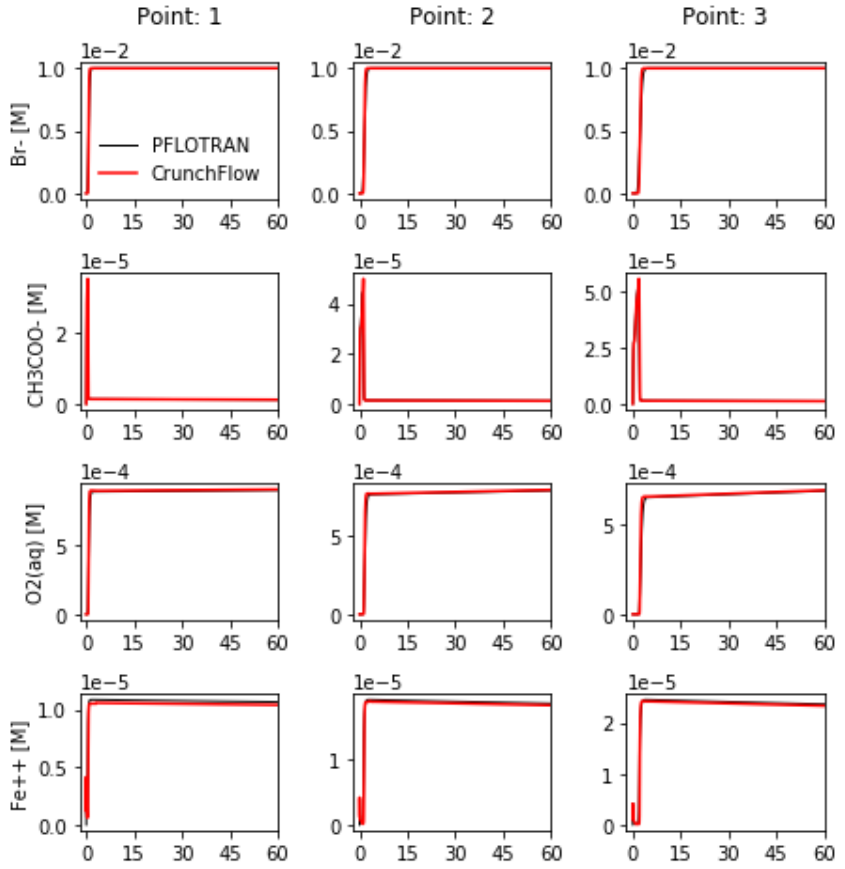
KBase Narrative
https://appdev.kbase.us/narrative/ws.39537.obj.1

Fine-Scale Use Case collaboration with SLAC SFA

Benchmarking PFLOTRAN and CrunchFlow for column experiments based on Riverton WY site.



Isothermal, saturated flow



- Reactive transport results matched under same flow conditions
- Slight difference in flow field due to viscosity calculations

SLAC collaborators:
Kate Maher, Tristen Babey

IDEAS WATERSHEDS

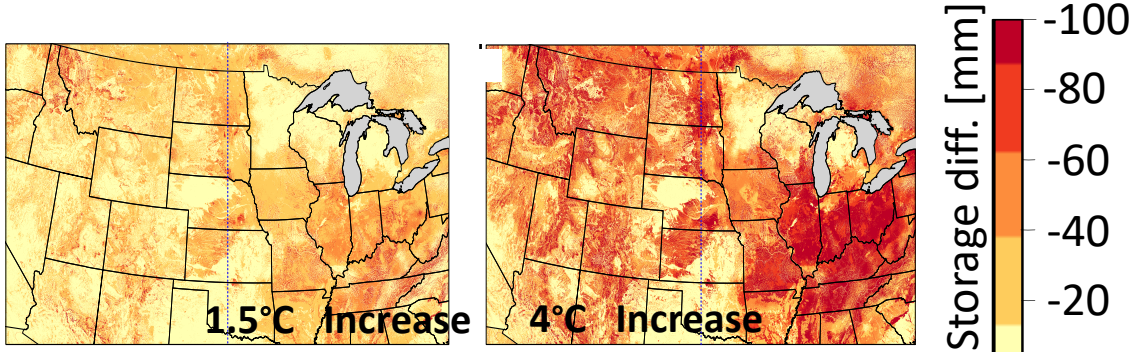
Research Activities on CONUS 1.0 Model

Reed Maxwell

Laura Condon

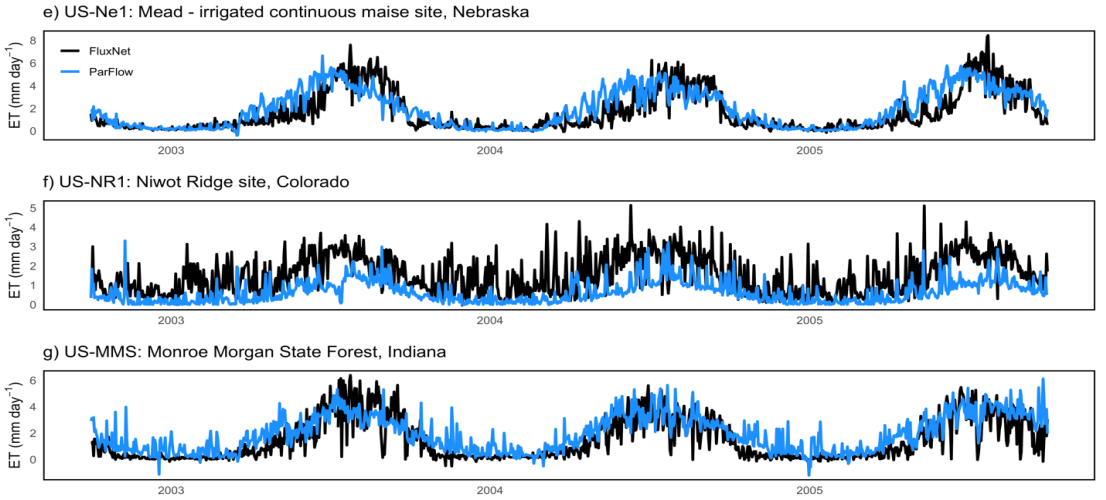
Warming simulations demonstrate increased aridification in North America and depleted ground water resources.

- Widespread lowering of water tables can have **dramatic impacts** on total water loss
- Even the modest 1.5C warming scenario resulted in losses 119,000 Million Cubic Meters (MCM): **4X Lake Powell** or 24% Lake Erie



Condon Atchley and Maxwell Nature Communications (2020)

Additional modern simulations with CONUS1.0 used to rigorously evaluate model performance and water balance



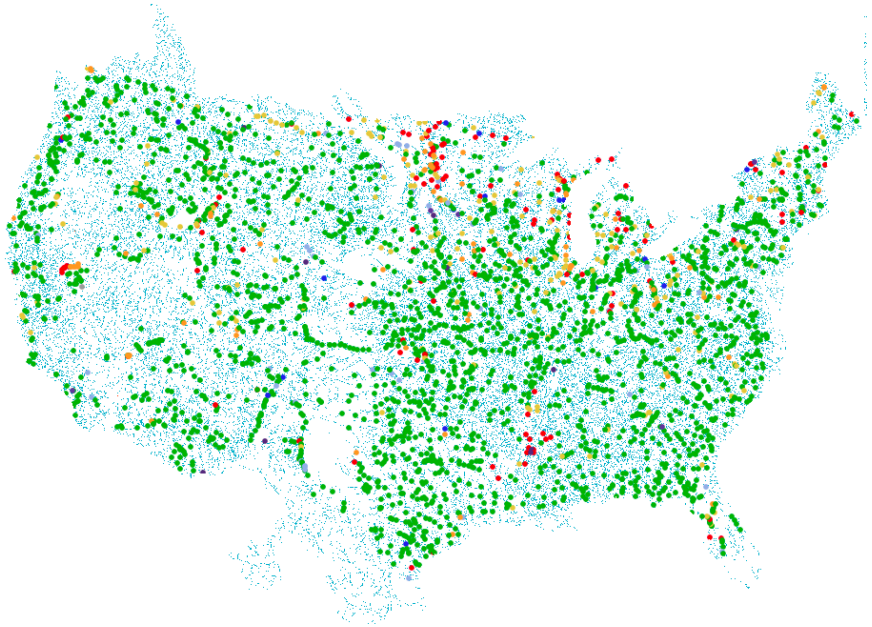
Examples of observed and simulated daily ET at three FLUXNET sites with complete observation periods during the simulation timeframe

Forester M.M. et al, In Prep, GMD

IDEAS WATERSHEDS

Research Activities on CONUS 2.0 Model

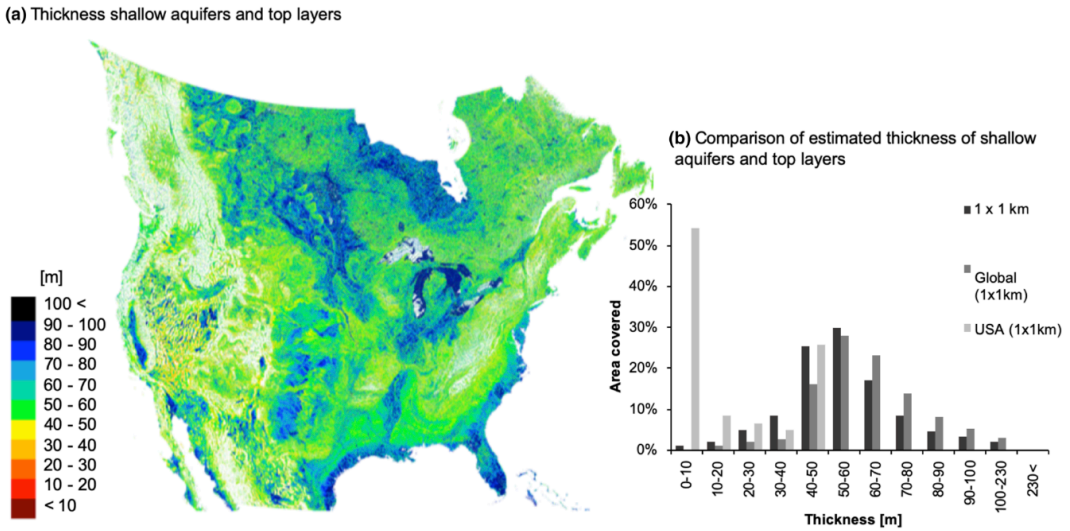
Topographic processing and overland flow testing



- Evaluating the streamflow network and adjusting to improve match between NHD, CONUS2.0 and gauge locations
- Testing topographic smoothing and river slope calculation options for runoff performance

Subsurface parameterization

- Developing a suited of subsurface parameterizations combining available data with hydrologic process understanding
- Testing steady state groundwater configurations

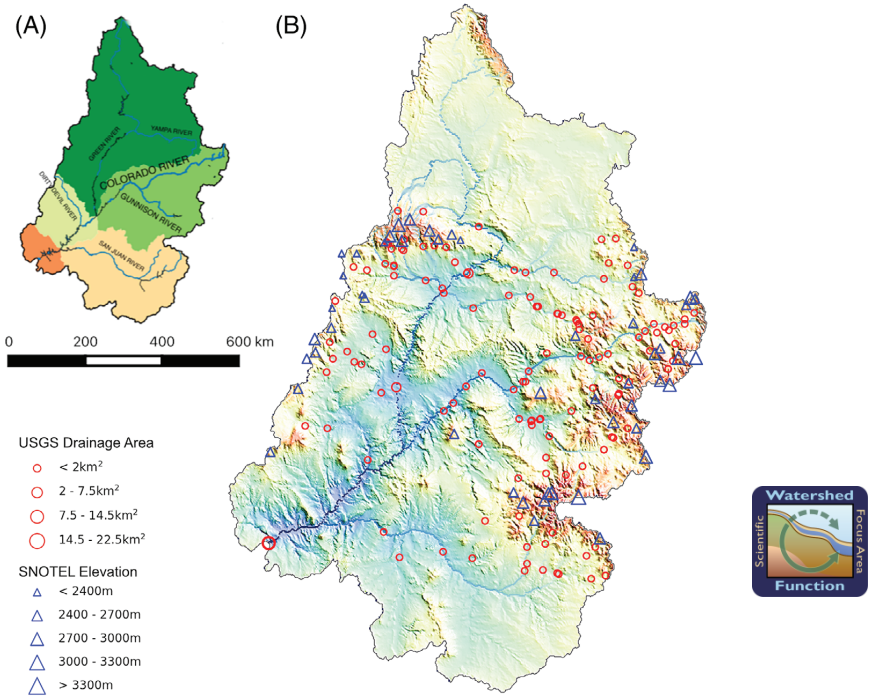


De Graaf, Condon & Maxwell, Hyper-Resolution Continental Scale 3-D Aquifer Parameterization for Groundwater Modeling, WRR (2020)

IDEAS WATERSHEDS

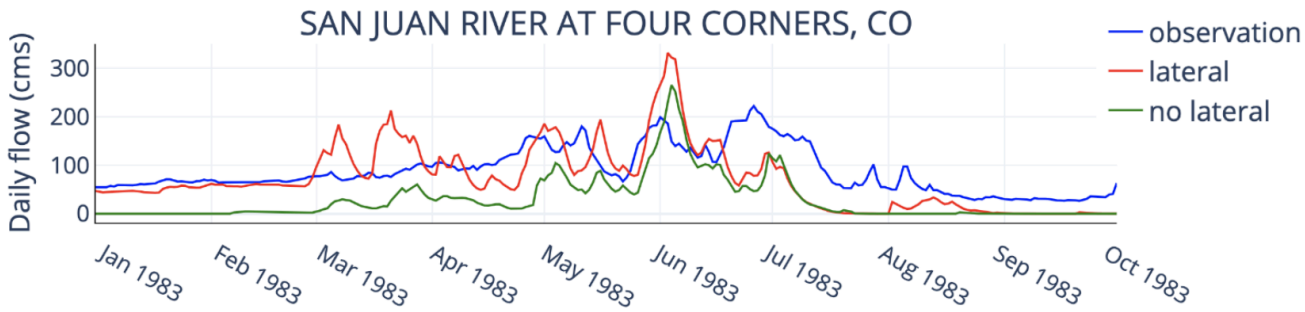
Research Activities CONUS sub-models and test-beds

Developing a numerical test-bed for the Upper Colorado River Basin leveraging sub-setting of CONUS models and simulations



Simulated four decades with ParFlow-CLM creating the first complete hydrology reanalysis of the UCRB

Lateral groundwater flow is important even for simulating flood conditions

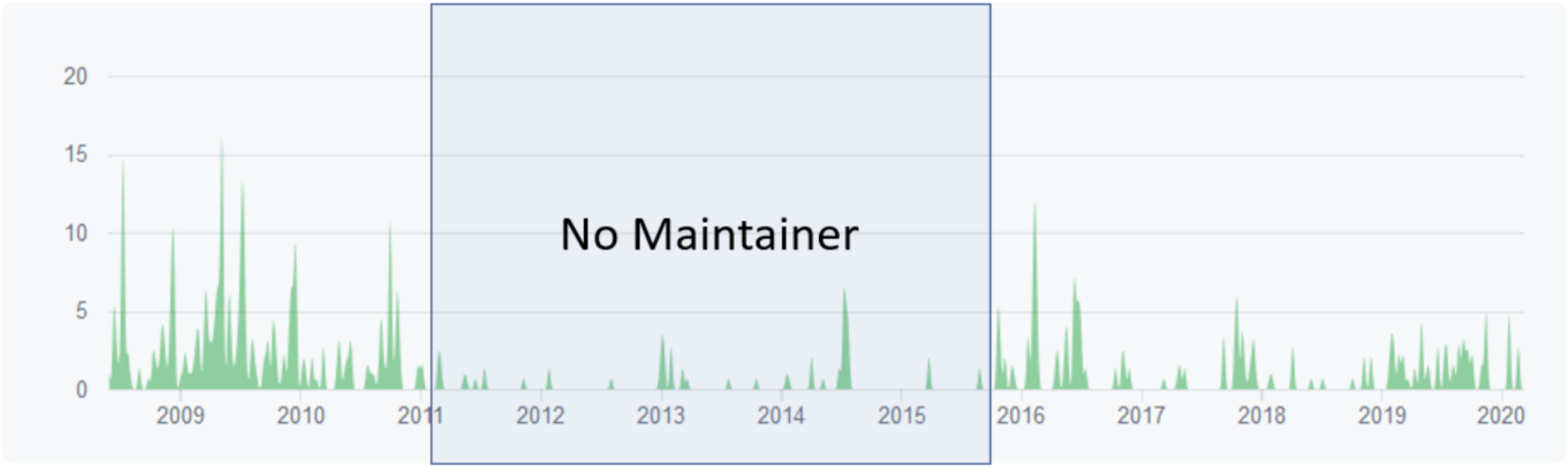


*Tran, H, **J Zhang,** JM Cohard, **LE Condon** and RM Maxwell, Simulating groundwater-streamflow connections in the Upper Colorado River Basin, Groundwater, 2020.*

Critical Role of the Code Maintainer for Sustainability and Productivity

Lead: Software Engineer

- The responsibilities of a code maintainer include,
  - reviewing and integrating ongoing development,
  - ensuring that project standards for coding practices and documentation are met
  - ensuring that testing is being done and bugs are fixed in a timely manner,
  - publishing trusted releases for users,
  - supporting an issue tracker to track bug reports and feature requests from users.
- Explored the important role of the code maintainer with ParFlow Team.
- Published BLOG article about maintainers Better Scientific Software
  - https://bssw.io/blog_posts/maintainers-drive-software-sustainability



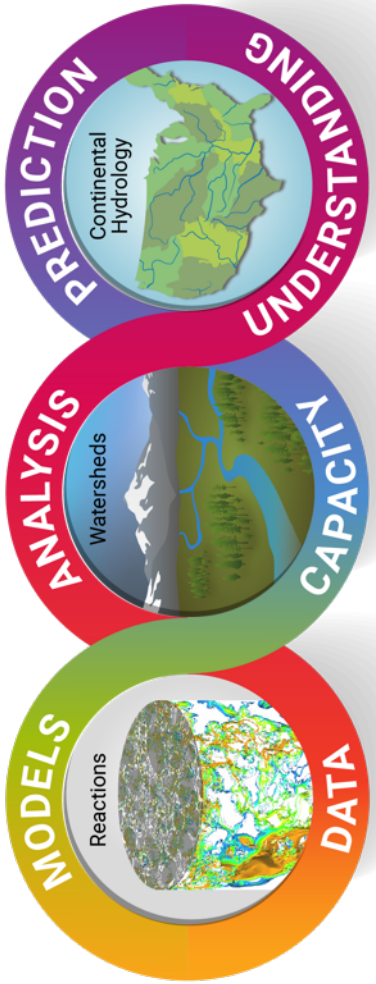
History of code commits to the ParFlow git repository ***showing a significant increase in commits during the periods with a maintainer.***

IDEAS WATERSHEDS

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