

# ExaSheds: Advancing Watershed System Science using Machine Learning and Data-Intensive Extreme-Scale Simulation

Dipankar Dwivedi, (LBNL), Ethan Coon (ORNL)  
Xingyuan Chen (PNNL), Ben Brown (LBNL), David Moulton (LANL),  
Scott Painter (ORNL), Carl Steefel, (LBNL)

# ExaSheds



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science



# Healthy watersheds are critical to water security

- Watersheds funnel rain and snowmelt to rivers where they can be used by municipalities, agriculture, and energy producers.



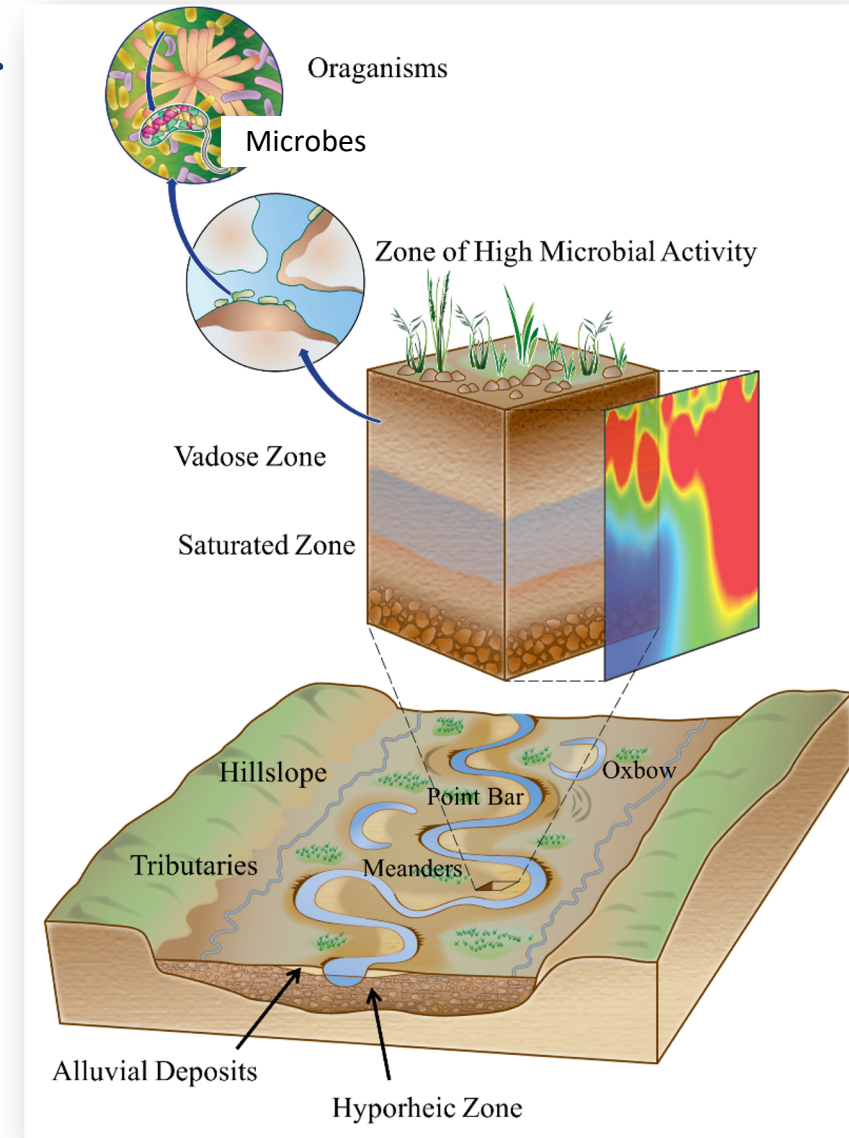
A predictive understanding of watershed function that is both predictive and mechanistic is required to ensure water security.

- Increases in contaminant and nutrient inputs
- Changing precipitation patterns and temperature



# Gaps

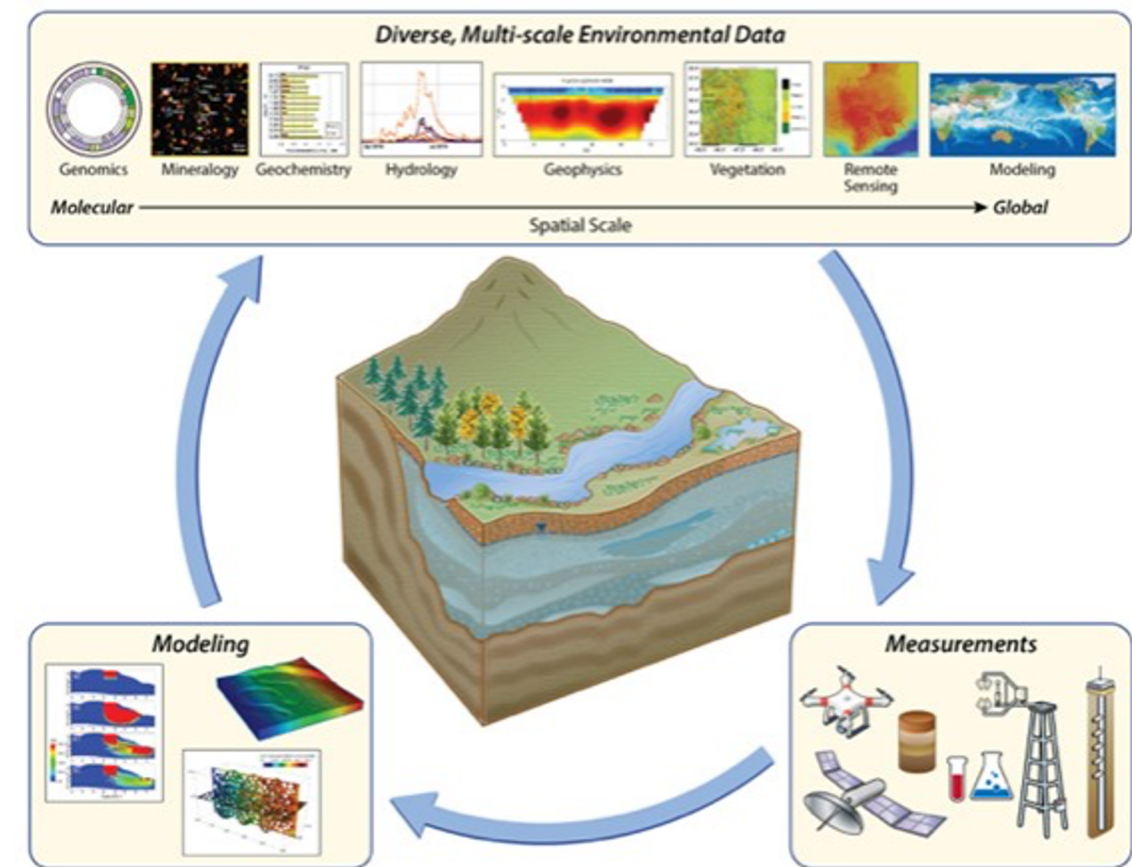
- Current generation **water quality modeling** tools for watersheds do not fully incorporate coupled multi-physics processes
- **Multi-scale character** of watersheds poorly represented
- **Real time data-model integration** is not presently considered, and rigorous UQ is neglected
- Mechanistic representations come with **large computational and characterization burdens**



# ExaSheds: Advancing computational watershed science with machine learning and advanced simulations

**5-year vision:** Hyper-resolution, process-explicit hydrobiogeochemical simulations **at river basin scales** taking full advantage of diverse and spatially extensive data and providing feedback to design of distributed networks

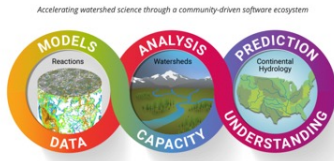
**Approach:** Combine modern data-driven approaches with advanced integrated surface-subsurface hydrological and biogeochemical models leveraging leadership-class computing facilities



EESA18-041

Varadharajan et al. (2018)

**Learning-assisted multiscale simulations**



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

ATS + Alquimia  
(code related development)

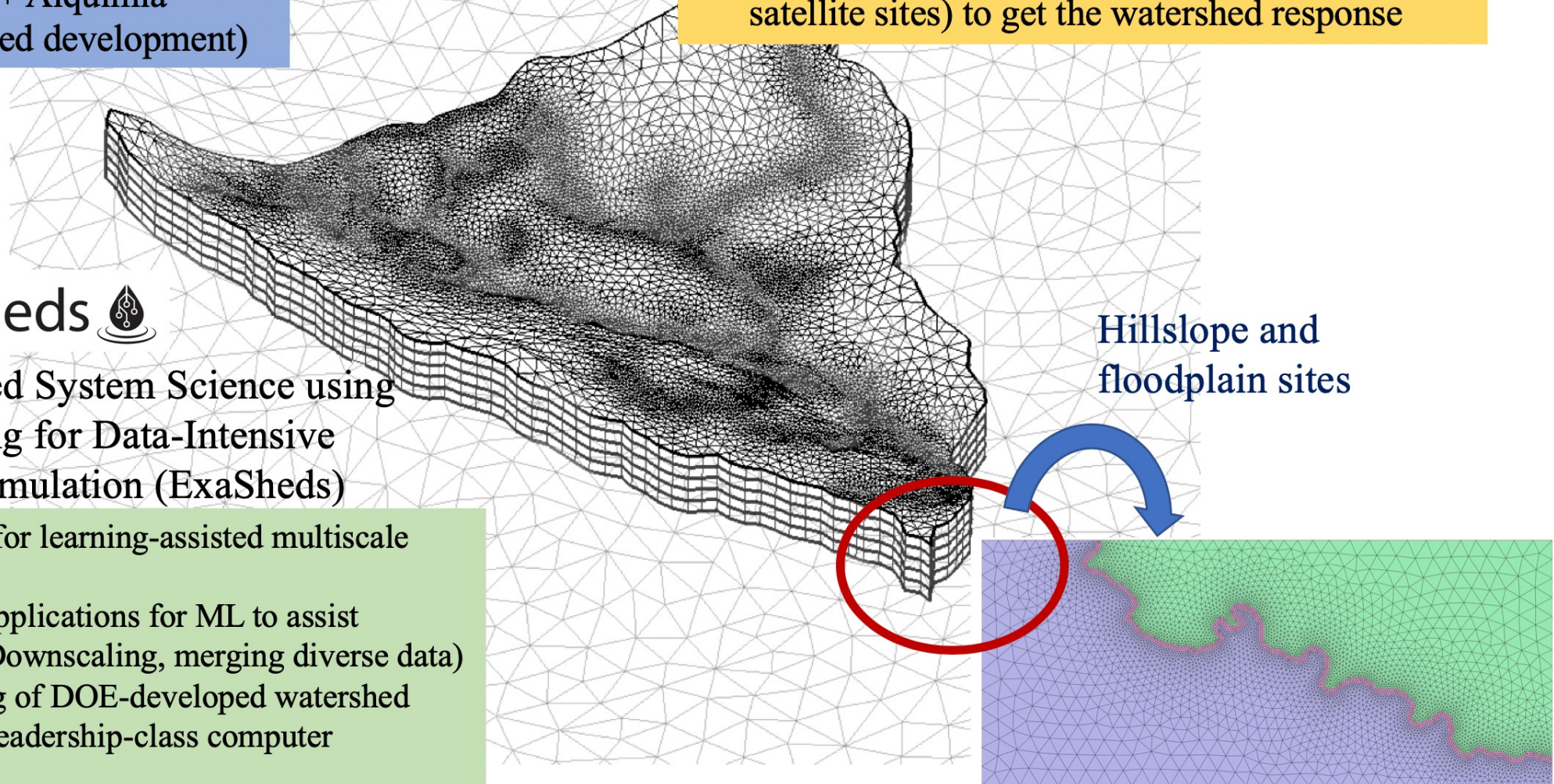
## SAWASC (SFA)

1. Develop Variable Resolution Meshes
2. ML-assisted bi-directional exchanges
3. Make use of zones (zonation approach)
4. Integrate subsystems (e.g., intensive and satellite sites) to get the watershed response

## ExaSheds

Advancing Watershed System Science using Machine Learning for Data-Intensive Extreme-Scale Simulation (ExaSheds)

- Explore strategies for learning-assisted multiscale simulation
- Explore example applications for ML to assist simulations (e.g., Downscaling, merging diverse data)
- Preliminary porting of DOE-developed watershed modeling tools to leadership-class computer architectures

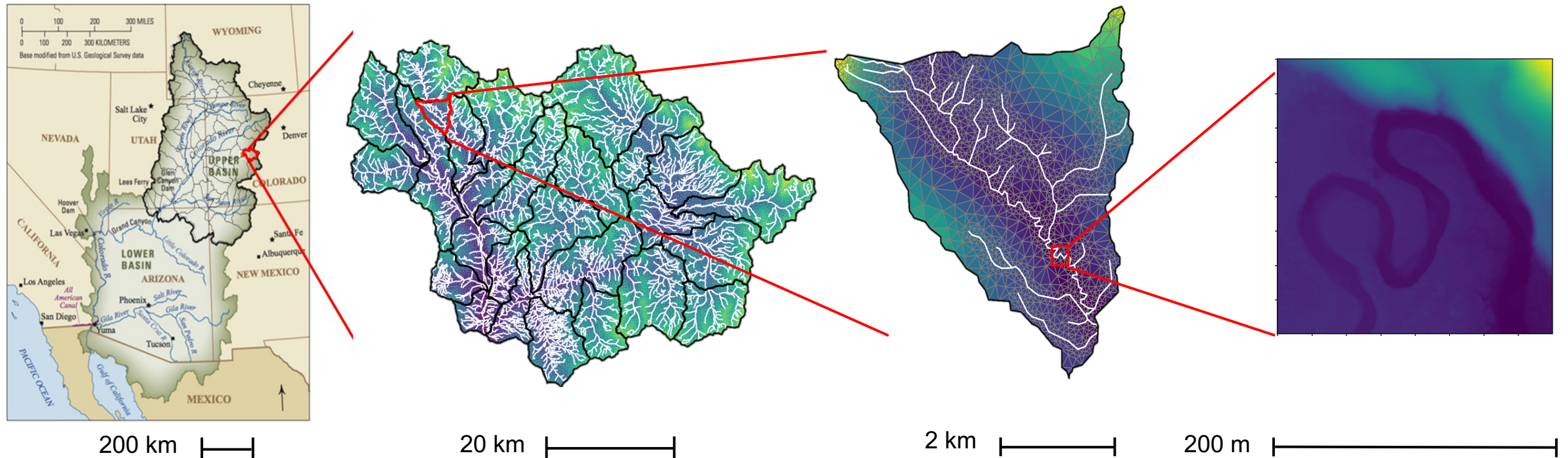


Hillslope and floodplain sites

# Learning-enabled Data Model Integration Across Scales

Data driving models across scales, from catchments to full-river basins.

- Digital elevation models: LIDAR → NED
- Soil databases: Geophysics → NRCS Soils
- Hydrography: LIDAR → NHD
- Meteorological data: Weather Stations → DayMet
- Land cover/vegetation: Mapping → NLCD
- Hyporheic exchange flux: Tracer experiments → NEXSS



**Machine learning approaches for integrating between and across scales.**