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IDEAS-Watersheds: Partnership with the Watershed Function SFA and Fine-Scale Reaction Network Activities

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The next phase of the Interoperable Design of Extreme-scale Application Software project (IDEAS-Watersheds) will focus on development and demonstration of modeling capabilities needed to further advance process-rich biogeochemical reaction network models and hydro- biogeochemical watershed models. In this presentation, we will discuss two activities within the project: (1) the partnership with the Watershed Function SFA to develop a multiscale modeling framework that will allow us to consider processes at different resolutions within the watershed and (2) the fine-scale activities in collaboration with the SLAC, ANL and LLNL SFAs to implement improved models and workflows for biogeochemical reactions.

The Watershed Function SFA seeks to determine how perturbations to mountainous watersheds impact the downstream delivery of water, nutrients, carbon, and metals. The vast study area of the East River Watershed, a representative mountainous watershed in the Upper Colorado River Basin, contains pronounced gradients in hydrology, geomorphology, or type of biome. This represents a challenge for models, especially for the aggregation of the system behavior across subsystems and scales. In this partnership, we are developing the software tools and workflows required to enable a multiscale framwork that relies on multiple resolution unstructured meshes to dynamically adjust the process resolution and efficiently perform the simulation over large spatial extents. Development is primarily based on the ATS with a specific emphasis in the newly available reactive transport capabilities. A critical aspect of the work is on the meshing tools (e.g. LaGriT, pylagrit) that support the generation of unstructured meshes with variable resolutions. Development of reaction networks to describe biogeochemical transformations is a central component of the SBR research. All SFAs in one form or another develop and use reaction models for aqueous complexation, surface complexation, mineral dissolution-precipitation, and microbially mediated reactions. In particular, the SLAC, LLNL and ANL SFAs focus on developing mechanistic models of biogeochemical transformations in subsurface environments at fine scales, using molecular, genomic, metabolic, solid-phase, and aqueous chemistry data. Collaboration with IDEAS-Watersheds focuses on two major aspects: (1) developing new approaches and workflows to incorporate new data and knowledge into the reaction models, including the derivation of reaction networks from metagenomics data and reaction parameters; and (2) implementing reaction models that reflect the new understanding in existing codes.