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Leveraging Software Interoperability and Benchmarking to Accelerate Model Development of Terrestrial Ecosystems - IDEAS Use Case 1

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To advance a robust predictive understanding of multi-scale terrestrial ecosystems requires representation and coupling of all relevant processes in models. There are various codes that are capable of quantifying hydrological and biogeochemical response across scales with slightly contrasting modeling approaches, but none of these can currently handle the full problem. In this presentation, as part of the overarching goal of **I**nteroperable **D**esign of **E**xtreme-scale **A**pplication **S**oftware (IDEAS), we demonstrate interoperability between codes to improve software and ultimately scientific productivity. In particular, we summarize two activities: (1) quantify the stream concentration-discharge at the Copper Creek (CC) sub- catchment and Lower Triangle Region (LTR) of the East River catchment to showcase a new level of spatial and time resolution as well as process fidelity in the modeling of multi-scale terrestrial ecosystems; (2) use model intercomparison to benchmark capabilities and build confidence in the model results.

The CC and LTR are located in the East River catchment, which is a study site of the Berkeley Lab's Watershed Function SFA, in southwestern Colorado. The CC is a high elevation sub-catchment which contributes flow to the East River approximately 25% annually, whereas the LTR encompasses complex geomorphic units such as floodplain, hill-slope, and meanders of the East River. ATS-AMANZI, which supports process-rich coupled simulations using Arcos multi-physics framework, is used to simulate integrated hydrological processes, winter snowpack, and follow-up snowmelt that influence stream chemistry at CC and LTR. The Alquimia interface, an interoperable interface designed to provide biogeochemical processes to flow/transport models, is used to represent geochemical processes including chemical weathering of rock and solute transport as well as mineral precipitation and dissolution in the models. Preliminary simulation results at CC and LTR show that hydrologic flow paths and groundwater residence times are key controls of stream concentration-discharge relationships.

Model intercomparison focuses on understanding differences in fluxes estimated by various reactive transport codes because of the distinctions in their abilities to handle structured vs. unstructured meshes. Here, we use ParFlow, ATS-AMANZI, and Chombo-Watershed to model complex and highly resolved topography encompassing two meanders of the lower East River catchment. ParFlow and ATS-AMANZI use structured and unstructured meshes, respectively, while Chombo-Watershed use embedded boundary adaptive mesh refinement (AMR) based package for creating meshes. Simulation results of integrated hydrology show confidence in model results by three codes. In addition, efforts are underway to benchmark biogeochemical processes for the same model domain.