

Authors: Lauren Foster¹, James Beisman¹, Reed Maxwell¹, Lindsay Bearup¹, Ken Williams², Rosemary Carroll³

¹Colorado School of Mines, ²Lawrence Berkeley National Lab, ³Desert Research Institute

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Development of multiple simulation capabilities to model hydrologic partitioning and biogeochemical cycling at the Berkeley Lab's East River Field Site

Berkeley Lab's Subsurface Biogeochemistry Watershed Function SFA seeks to develop a mechanistic understanding of coupled climate-hydrological processes that underlie the ability of mountainous watersheds to retain and release water, nutrients, carbon, and metals. Development of simulation capabilities that describe both flow of water and reactant transformations are sorely needed, as are numerical experiments that predict their response to system disturbance and climate-induced changes. Here, we present two new simulation capabilities utilizing the physically based hydrologic model ParFlow and developed to investigate complexities from the biogeochemical scale up to watershed partitioning: 1) a highly resolved, fully integrated hydrologic model and 2) a new reactive transport model, ParFlow.RT.

The most highly resolved, (2.76M, 10m cells over a 273km² domain), fully parallelized, integrated watershed model from the subsurface through the land surface was built for Berkeley Lab's East River SFA Watershed Study Site. This model provides a platform for numerical experiments studying the influence of climate and vegetation change on hydrologic partitioning and biogeochemical feedbacks. The model was driven to dynamic equilibrium then driven by spatially variable estimates of meteorology at hourly intervals. Model output is compared with field observations to answer questions posed by the Watershed Function SFA. In tandem with field manipulations, these simulations help develop a robust understanding of environmental changes on hydrology. This model is the most highly resolved integrated watershed model in the world to date, allowing for experiments to probe the limits of computational hydrology.

In natural subsurface systems, total elemental fluxes are heavily influenced by areas of disproportionately high reaction rates. These pockets of high reaction rates usually occur at interfaces, such as the hyporheic zone, where a hydrologic flowpath converges with a chemically distinct flowpath or a reactive substrate. Understanding these highly reactive zones is integral to the accurate quantification of nutrient fluxes and biogeochemical cycling in natural systems. Reactive transport simulations can provide information about controls in these highly reactive zones. We have developed a new reactive transport model, ParFlow.RT, by coupling the parallel flow and transport code ParFlow with the geochemical engines of both PFLOTRAN and CrunchFlow. The coupling was accomplished via the Alquimia biogeochemistry library, which provides a unified interface to several geochemical models. Here, we present the details of this new model, and the results of biogeochemical simulations of the Berkeley Lab's East River field site outside of Gothic, CO.