Watershed Function Simulation and Aggregation

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Watershed hydrological processes mediate a wide range of biogeochemical interactions, ranging from vegetation growth to elemental and nutrient cycling to contaminant fate and transport. However, there are huge uncertainties associated with predicting how watersheds will respond to such perturbations (e.g., droughts or floods) at space and time scales relevant to the management of environmental and energy strategies. Complementing modeling activities focused on intensive study sites in other components of the Watershed Function SFA, the Watershed Reactor effort aims to understand and predict the aggregated behavior of the system affected by coupled hydrological, energy, and biogeochemical processes. One important challenge is the resolution of hot spots (spatially focused zones of intense hydrological or biogeochemical activity) and hot moments (transient events with potentially outsized impact on system function). As an example, hydrological flow and biogeochemical processes may generate meter scale gradients in concentration in reactive floodplains, and these may need to be captured in models to accurately represent fluxes. Similarly, hillslope processes may be affected by small scale variations in vegetation and slope and weathering depth, all impacting fluxes to the river system. To address these potentially outsized impacts on river quality, we are developing HPC simulations using the IWaSE (IDEAS Watershed Software Ecosystem) for the Lower Triangle and Copper Creek within the East River watershed. Using the Amanzi-ATS package for flow and transport within IWaSE, we make use of variable resolution unstructured grids that focus resolution in the floodplains and other zones where hydrologic and/or biogeochemical hot spots can develop. In addition, we use high resolution hydrological modeling based on the ParFlow-CLM software to calculate travel time distributions for surface and subsurface water within the East River watershed. These are used by both the Han-SoMo bioreactor model, and to analyze the partitioning of water between the surface and subsurface by comparing simulation results with isotopic measurements of river water at various places within the watershed. In Copper Creek, our focus initially is on capturing stream discharge, with the ultimate objective of using reactive transport capabilities within IWaSE to address the question of how variable depth weathering fronts (i.e., \textsuperscript{16}O\textsubscript{2} and CO\textsubscript{2} driven) impact watershed biogeochemical fluxes.