Multiscale Simulations of Hydrological and Biogeochemical Processes from the Pore to Ecosystem Scales

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A major challenge in hydrological and biogeochemical modeling is the disparity between the spatial and temporal scales at which processes are fundamentally understood and quantified (e.g., pore scales, seconds to days) and the practical applications of these processes in larger-scale modeling (ecosystems to global scales, days to years). In this presentation, we will describe multiscale simulation approaches to bridge this disparity. First, a unified multi-scale model (UMSM) has been developed that uses a single set of mathematical equations to simulate moisture migration and materials fluxes at different scales under both saturated and unsaturated conditions. The UMSM can directly incorporate mechanistic biogeochemical reaction network in soils at the pore-to-core scale. It also allows the pore-to-core scale biogeochemical processes to be seamlessly scaled up to the ecosystem scale through effective parameterization. Coupled to a PNNL-developed reaction-based community land model, the UMSM can be tested against field flux measurements and thus evaluate the transition of reaction rate expressions and parameters from the relatively fine grid scale to coarse grid scale.

Two examples will be provided to demonstrate the capabilities of the UMSM from the pore to ecosystem scales in simulating hydrological processes. Examples include modeling water flow and saturation condition at the pore-to-core scale, and simulating ecosystem-scale hydrological processes at the Disney Wilderness Preserve eddy covariance site. Finally, we describe larger-scale analyses examining how well soil-to-atmosphere C fluxes can be predicted from simple measurements, and test the resulting relationships against both observed and modeled (CMIP5) data.

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