Presentation Abstracts

The GEWaSC Framework: A Genome-Enabled Approach to MultiScale Modeling of Coupled Microbial Biogeochemical and Hydrological Processes

Carl Steefel (CISteefel@lbl.gov) - Lawrence Berkeley National Lab (PI), E.L. Brodie, S.B. Yabusaki, E. King, N. Bouskill, S. Molins B. Arora, U. Karoz, N. Spycher, R.M. Maxwell, A. Navarre-Sitchler, J. Beisman; Project Leader: Susan Hubbard; (Co-PIs).

In order to improve our ability to predict the effect of climate change on carbon and nutrient cycling, we are developing a genome-enabled multiscale reactive transport framework (GEWaSC) that couples microbial composition, competition, and activity to biogeochemical processes and the hydrologic cycle at the watershed scale. This new simulation capability goes beyond conventional watershed models by ultimately integrating surface processes (e.g., those taking place in the soil and surface waters) with the subsurface flow and transport in a formal manner to provide a complete description of the biogeochemistry of carbon and nutrient cycles within a catchment. A novel feature of the modeling approach is the coupling of microbial functional groups (guilds) inferred from trait-based models, parameterized using site-specific 'omic data, with a comprehensive simulation of the biogeochemical network. The composition of these guilds is a function of the organisms' physiological traits along with environmental, physical and geochemical conditions that exist across flow paths to create 'hot spots' of activity. Our approach models the rate of nutrient uptake and the thermodynamics of coupled electron donors and acceptors to predict the energy available for respiration, biomass development and exo-enzyme production. Each group within a functional guild is parameterized with a unique combination of traits governing organism fitness under dynamic environmental conditions.

Initial model application is to biogeochemical and microbial dynamics within the Rifle Flood Plain system, a component of the greater Colorado River system. Preliminary work focuses on carbon and nitrogen cycling at the Rifle Flood Plain site and is being carried out at four scales: 1) development of microbial trait-based (EcoTrait) simulation capabilities based on genomic studies and designed for integration with flow and transport models, 2) 1D and 2D simulations along a transect through the Rifle Flood Plain with both vadose zone and groundwater contributions, 3) 3D simulations of the Rifle Flood Plain focusing on seasonal oxygen consumption in upstream and Naturally Reduced Zones (NRZ), and 4) simulations of the greater Rifle watershed, with a focus on the contribution of upland groundwater fluxes and the role of heterogeneities in establishing the sub-oxic status of the aquifer. Initial modeling and data analysis emphasize the important role of the NRZ (or "biogeochemical hotspots") in mediating the redox status of the alluvial plain aquifer, with the important role of microbially-mediated carbon and sulfur oxidation indicated by elevated fluxes of inorganic carbon and isotope ratios of groundwater sulfide.