

Genomes to Watershed LBNL SFA 2.0: Modeling Microbial Community Dynamics with Genome-Informed Trait-Based Models

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The Genomes to Watershed SFA 2.0 is focused on addressing uncertainties in how climate or land-use-induced changes in hydrology and vegetation will affect subsurface carbon flux, the spatial and temporal distribution of flow and transport, biogeochemical cycling, and microbial metabolic activity. Here we report on the development of a Genome-Enabled Watershed Simulation Capability (GEWaSC), which provides a predictive framework for understanding how genomic information in a subsurface microbiome affects biogeochemical watershed functioning, how watershed-scale processes affect microbial function, and how these interactions co-evolve. In recent years, cultivation-independent approaches have further elucidated knowledge of microbial functional diversity within the subsurface. With the emerging capability to reconstruct thousands of genomes from microbial populations using metagenomic techniques and gene expression data, there is a need to develop an understanding of how these metabolic blueprints influence the fitness of organisms and how populations emerge and impact the physical and chemical properties of their environment.

We have developed a hybrid trait-based reaction transport model of microbial activity (BioCrunch) that simulates coupled guilds of microorganisms. Guild selection is driven by traits and physiological properties extracted from large-scale assembly of metagenome data. Metagenome information is also used to complement our existing biogeochemical reaction networks and contributes key reactions where biogeochemical analyses are equivocal. Our approach models the rate of nutrient uptake and the thermodynamics of coupled electron donors and acceptors for a range of microbial metabolisms including heterotrophs and chemolithoautotrophs. Exogenous substrates fuel catabolic and anabolic processes, with the proportion of energy used for each based upon dynamic intracellular and environmental conditions. In addition to biomass development, anabolism includes the production of key enzymes, such as nitrogenase for nitrogen fixation or exo-enzymes for the hydrolysis of extracellular polymers. This internal resource partitioning represents a trade-off against biomass formation and results in microbial population emergence across a fitness landscape. We use this model in simulations of biogeochemistry within the Rifle floodplain system, a component of the greater Colorado River system. Simulations and metagenomic/metatranscriptomic observations identify a number of functional guilds with chemolithoautotrophic lifestyles that appear to be important in mediating elemental cycling within aquifer biogeochemical hotspots. In addition, key processes regulating aquifer oxygen concentrations during seasonally fluctuating water table regimes are explored.