Title: **An Iterative Approach to Linking Genome Scale Metabolic Models with Reactive Transport Simulation**

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Project Abstract:

Critical zone hydrobiogeochemical systems play a key role in carbon and water cycling, which makes them extremely important both scientifically and economically. The “bio” component of these systems is known to drive many core processes, but is often treated as a black box when integrated with large scale simulations due to the challenge of linking across domains and scales. As a result, these simulations may fail to capture complex interactions between the critical zone microbial community and the surrounding environment. We have previously demonstrated a means by which genome scale metabolic models built in KBase may be used to inform PFLOTRAN reactive transport simulations in order to better define the chemistry of microbe-driven reactions. Flux balance analysis performed in KBase is used to describe the reaction stoichiometry used in PFLOTRAN, so the reactions are based on actual microbial metabolisms rather than rule-of-thumb approximations. We now expand this approach to include iteration between the metabolic and reactive transport models so that the two components evolve alongside and in response to one another. Thus, we can predict how the system will behave over time as limiting resources change and various nutrients are exhausted or newly created. For demonstration purposes, we have applied this approach to nitrogen cycling in hyporheic zone sediments. The initial model definition is based on real-world samples collected from Hanford 300 reach sediments. This includes a simplified microbial system based on metagenomic analysis and chemistry defined based on geochemical and metabolomics analysis. With each iteration, the chemical profile simulated using PFLOTRAN is provided to KBase as a new media formulation and used to generate new flux balance analysis solutions, which then in turn provide new stoichiometries for the microbe-driven reactions. This approach allows our simulations to better capture ongoing system dynamics as well as short-term responses to perturbations.