Integrating BER Facilities and Resources for Multi-Omics to Reactive Transport Modeling Workflows

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https://www.kbase.us/multiscale-microbial-dynamics-modeling/

Microbial community dynamics strongly affect the function of natural ecosystems, but their impacts are difficult to quantify and predict because of challenges related to the wide range of spatial and temporal scales and multidisciplinary integration. Multiple BER user facilities and resources, spanning research programs across both divisions of BER, can be brought to bear on these challenges. This potential was demonstrated in a week-long summer school organized in July 2020 by the Environmental Molecular Sciences Laboratory (EMSL) in close collaboration with KBase, JGI, ESS-Dive, WHONDRS, and individual researchers funded by BER programs. The BER community came together to construct a multi-omics to reactive transport modeling workflow, much of it embodied within the KBase platform, and to demonstrate its use through application to community environmental datasets developed through the WHONDRS consortium employing JGI, EMSL, ESS-DIVE and other BER resources.

This multiscale approach to microbial dynamics modeling combines environmental metabolomics and metagenomics data to formulate complex microbial community reaction networks. These can be solved using metabolic modeling methods such as flux balance analysis, resulting in reaction models and rate formulations that can be incorporated into ecosystem-scale reactive transport codes such as PFLOTRAN. Alternative pathways through the workflow were also demonstrated in the summer school, including the use of thermodynamics-based theories to define reaction rates from elemental composition of organic matter in natural samples provided from high-resolution metabolomics datasets. Public presentations and demonstrations were provided to over 500 globally distributed participants, and 28 selected students participated in intensive hands-on sessions using WHONDRS datasets. Course materials are openly available on KBase at the URL above.