IDEAS-Watersheds PNNL SFA Partnership: Multi-Scale River Corridor Hydrobiogeochemical Modeling

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BER Program: SBR

Project: IDEAS-Watersheds

Project Website: https://ideas-productivity.org/ideas-watersheds/

Project Abstract:

The IDEAS-Watersheds partnership with the PNNL SFA focuses on developing general workflows that leverage community software ecosystem to advance river corridor hydrobiogeochemical research, which will in turn be made available to the broader community. In the past year, we have developed an entire modeling pipeline from metagenomes to biogeochemical models and to reactive transport models, leveraging the DOE's KBase modeling platform. The core pipeline of the workflow include: 1) metabolic network construction from metagenomes; 2) identification of key substrates by metabolic pathway analysis; 3) development of stoichiometric and kinetic forms of biogeochemical reactions for the key substrates identified in the previous step, and 4) incorporation of the biogeochemical reaction model into a one- dimensional reactive transport model using PFLOTRAN. The workflow also allows optional steps that provide the methods for incorporating other omics datasets (such as metatranscripts, metaproteomics and metabolomics) when available. We have prototyped the workflow as KBase Apps using KBase Software Development Kit (SDK): one for translating chemical compositions from FTICR-MS into biogeochemical reaction models, and one for 1-D reactive transport modeling using PFLOTRAN. A KBase narrative using SFA example data has been made available to demonstrate the use of the Apps.

In collaboration with the National Center for Atmospheric Research (NCAR), we have also developed a data assimilation framework by linking Data Assimilation Research Testbed (DART) with PFLOTRAN. In addition to the access to various forms of ensemble data assimilation methods that are provided by DART, we have also implemented an ensemble smoother option that suits typical parameter estimation needs in SBR watershed research. We will further deploy DART-PFLOTRAN on KBase modeling platform as an App to facilitate assimilation of lab experimental data to estimate reaction kinetics parameters, thus enabling the ModEx iterations for batch- and column-scale biogeochemical predictive modeling. We have been working closely with other SBR SFAs to test the workflow design to broaden the science impacts.