IDEAS-Watersheds: Cross-cutting view and Integration– Workflows and Fine-scale activities

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BER Program: SBR

Project: IDEAS-Watersheds (LBNL)

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

Project Abstract: IDEAS-Watersheds is organized around six Research Activities driven by the Partnerships that the project has established with the different SBR SFAs and the CONUS simulation platform. However, it is in the sharing and contrasting of approaches between Partnership activities that the project meets the goal of advancing software development methodologies and engagement in the growing community-driven software ecosystem. In this poster, we provide a cross-cutting perspective of the IDEAS-Watersheds project along 3 themes that are used for project integration: geochemical modeling, workflows, and multi-scale approaches.

Geochemical modeling in IDEAS-Watersheds relies on PFLOTRAN and CrunchFlow. These codes are available as stand-alone codes as part of the software ecosystem but also as geochemical engines in other codes via the Alquimia interface. As part of IDEAS-Watersheds work, Alquimia has now been implemented in Parflow. We are also working on developing an Alquimia interface to PHREEQc. After this is complete, Amanzi-ATS and Parflow will be able to access either PFLOTRAN, CrunchFlow and PHREEQc.

The PNNL partnership has developed a new workflow that builds an entire modeling pipeline from metagenomes to biogeochemical models and to reactive transport models, leveraging the KBase modeling platform. The one-dimensional reactive transport component of the workflow has been tested on a column experiment in a natural reducing zone in collaboration with the SLAC SFA. The dataset is used to perform reactive transport benchmarking between PFLOTRAN, CrunchFlow and PHREEQC.

Different multiscale approaches are being developed for river-corridors that range from multi- resolution meshing to travel time-based approaches to represent exchanges between stream and the hyporheic zone. We contrast the workflows required to go from the river corridor data, to meshing the multiscale domains to performing the simulations. This is the first step towards an formal intercomparison between the different multiscale approaches.