Linking Molecular Characterization with Continuum Reactive Transport Modeling

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BER Program: ESS

Project: **IDEAS-Watersheds**

Project Website: https://ideas-watersheds.github.io/

Project Abstract:

The IDEAS-Watersheds focuses on developing flexible modeling capabilities and workflows through contributions to a community-driven software ecosystem that advance hydrobiogeochemical research in watersheds and river corridors.These contributions are in turn made available to the broader community. For example, we have developed a modeling pipeline from molecular characteristics, such as organic carbon speciation, to biogeochemical models and to continuum reactive transport models. Leveraging the DOE's KBase modeling platform, we have prototyped the two key steps of this pipeline as KBase Apps using the KBase Software Development Kit: one for translating chemical compositions from FTICR-MS into biogeochemical reaction models, and one that takes those reaction models and sets them up as 1-D reactive transport models with PFLOTRAN. After testing those new reaction networks and kinetics, which were informed by the organic carbon speciation, in PFLOTRAN in batch and column configurations, we incorporated those reaction models in ATS-PFLOTRAN for coupled hydrologic and biogeochemical modeling at the American River watershed. We used this coupled watershed model to investigate water, energy, and solute fluxes across the river-groundwater interface. The biogeochemical hot spots and hot moments within the river corridors are found to be strongly influenced by riverbed properties and flow conditions, and hence, influenced by variations in land use, hydrogeology, climate, and disturbances. This pipeline can be extended to allow the incorporation of other omics datasets (such as metatranscripts, metaproteomics and metabolomics) when they become available. We have shared our KBase narrative examples with the broader community to enable leveraging the pipeline in hydrobiogeochemical studies on other watersheds and river corridors. Finally, we note that the

ATS-PFLOTRAN coupled watershed model is an example of interoperable model development, where generic interfaces such as the Alquimia biogeochemistry interface library, extend the capabilities available from single codes in the software ecosystem by bringing their complementary capabilities together.

Progress Toward Scale-consistent Watershed Reactive Transport Models

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Project Abstract:

Most watershed-scale models focus on hydrological processes with limited capacity to represent the complex biogeochemical processes that control the efflux of greenhouse gases and the waterborne exports of carbon, nutrients, and trace metals. The IDEAS-Watersheds project in partnership with multiple watershed Science Focus Areas has been addressing that capability gap by extending parallel spatially resolved integrated surface/subsurface hydrology models to include reactive transport. The new capability addresses the central modeling challenges: coupling reactive transport across the surface and subsurface spatial domains, and tractably representing the effects of fine-scale biogeochemical phenomena without resorting to ad hoc upscaling. Those advances were enabled by software capabilities advanced by the IDEAS project including new approaches for multiphysics model coupling, mesh infrastructure that allows for multiple coupled meshes, and the application programming interface Alquimia, which provides hydrology codes access to widely used biogeochemical codes.

The Advanced Terrestrial Simulator (ATS) has been extended to couple multicomponent reactive transport across the surface water and subsurface domains (Molins et al., 2022). The integrated model has been used to investigate the response of the Copper Creek subwatershed in the East River, Colorado, Watershed over a ten-year period (Xu et al., 2022). Current modeling efforts focus on the Lower Triangle region to understand the processes affecting nitrogen exports with consideration of spatially-distributed watershed properties.

We have also developed a novel multiscale modeling approach (Jan et al. 2021) to represent the watershed-scale effects of biogeochemical transformations within small-scale biogeochemical

hotspots. We have implemented this model in ATS, used it to estimate model parameters from stream tracer tests (Rathore et al. 2021), demonstrated it on East Fork Poplar Creek Watershed and the Portage River Basin (Jan et al. 2021), and developed the workflow to build watershed-scale models from online data sources. We plan to extend the model-building workflow to improve estimates of hyporheic exchange flows using classification of hydrogeomorphic features.

These are first-of-a-kind capabilities that consider surface and subsurface reactive transport as an integrated multiscale system, thus improving representations of dynamic surface/groundwater exchanges, allowing for different reaction systems in the surface and subsurface, and avoiding *ad hoc* upscaling. We have plans to include additional watershed processes and integrate these new capabilities to provide a scale-consistent watershed reactive transport modeling tool that can be used to advance understanding of watershed hydro-biogeochemical function.

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Title: **National datasets and workflows for integrated hydrologic modeling across the US**

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Project Abstract:

The ParFlow-CONUS simulation platform has been in ongoing development for a decade and spans input data, several decades' worth of simulations, and comprehensive analysis tools to make the input and output data publicly available. This work has resulted in many publications that have advanced both technical capabilities for large-scale simulation, as well as scientific understanding of continental-scale hydrologic interactions including how transpiration and groundwater are linked, how the US' legacy of groundwater pumping has impacted the rest of the hydrologic cycle and how climate change may impact our groundwater resources both regionally and locally). Work is now focused on version 2 of the model (CONUS2.0) which expands from version 1 to cover the entire drainage area of the contiguous US. Over the last year we have published several publications that detail new national dataset development (Zhang et al 2021; Steyaert et al 2022), model intercomparison with the US National Water Model (Tijerina et al 2021), and a detailed evaluation of long-term version 1.0 simulations (O'Neill et al 2021).

Key to the successes of the ParFlow-CONUS platform are interoperable workflows that facilitate data and model development. While the static inputs to the model are small, forcing datasets for CONUS2.0 are much larger (~50TB in size) and the simulation outputs are expected to be almost 1PB. These large datasets have not only taken years to develop but are too large for traditional analysis approaches, and required our team to develop custom reproducible workflows in tandem with the dataset creation. To manage these large data sets and ensure the community can access them in practical ways, we are leveraging a dedicated datacenter (the Princeton Hydrologic Data Center, or PHDC) was constructed as a platform to store and serve these community resources.

In addition, our team has built subsetting workflows which have been used to construct regional models of the Upper Colorado (e.g. Tran et al 2022) and the Delaware-Susquehanna basins and will be available for the ESS community to use in their work.

This presentation will highlight the data-workflow-integration for high resolution continental- and regional-scale community model development and recent CONUS 2 accomplishments. National-scale model input datasets combine multiple sources and involve rigorous testing over both the entire CONUS 2 domain and subsets of it. The development of these data and how they improve the CONUS 2 simulation results will be discussed.

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