Title: **Accelerating Local to National Watershed Science through the IDEAS-Watersheds Software Ecosystem**

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Project Abstract:

Flexible workflows that enable scientists to easily integrate field and lab data with their conceptual model development and analysis are paramount to advancing our scientific understanding of watersheds. Such workflows include pre-processing of site data for model setup, parametric sensitivity analysis and parameter estimation, and subsetting of model output for use in subgrid models and analysis of model performance. The IDEAS-Watersheds open-source community driven software ecosystem provides the fundamental building blocks for these workflows as it includes workflow tools such as the pre-processing tools TINerator, PriorityFlow and Watershed Workflow, which prepare watershed data for use in models. In this poster we highlight two applications of workflow tools to hydrological modeling performed using codes in the IDEAS Watersheds software ecosystem.

First, an integrated watershed model has been developed for American River watershed (ARW) within the Yakima River Basin (YRB) by leveraging a community workflow in Jupyter notebooks that generates unstructured meshes and prepare ATS input files from multiple data sources, such as USGS NHDplus, NRCS land cover data products, USDA soil maps, and others. Long term (1997-2020) ATS model simulations have produced stream discharges at the ARW outlet that better match observations at the USGS stream discharge at the outlet than the more empirical SWAT simulations. The evapotranspiration (ET) and snow water equivalent (SWE) dynamics simulated by ATS show good agreement with MODIS ET and SWE data products. Watershed models were also developed for the Upper Colorado River Basin and the Delaware-Susquehanna Basin using the ParFlow CONUS model. We leveraged the capabilities and the new ParFlow-Python interface to subset these domains from the CONUS2.0 model. We ran ensembles of simulations across both domains testing a suite of subsurface parameterizations. We compared simulation output to USGS stream gauges and groundwater wells to evaluate

model performance across a range of hydrogeologic configurations. These test beds informed our final national scale parameters and provided a testing ground for transferable watershed workflows.

These examples highlight how flexible workflow tools enable hydrological modeling across scales as part of a software ecosystem that also includes the necessary process-based simulators.

Title: Interoperable and Reusable Software Enables Reactive Transport Modeling at Watershed Scales

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Project Abstract:

Although reactive transport modeling (RTM) has a long history and proven value in advancing mechanistic understanding of hydro-biogeochemical processes at small scales, application of reactive transport models at the large spatial scales needed to advance understanding of watershed function is relatively rare. Central among the many challenges in bringing RTMs to the watershed scale are the large computational demands, the complementary roles played by surface and subsurface systems, and the multiscale nature of hydrological and biogeochemical interactions. We present examples of how the IDEAS-Watersheds project is advancing an ecosystem of interoperable and reusable software that enables modelers to meet those challenges. The integrated surface/subsurface hydrology code Amanzi-ATS [1] has been extended [2] to model fully coupled reactive transport in shallow surface waters, the vadose zone, and groundwater. A key enabling technology is the Alquimia interface [3], which makes it possible for ATS to access capabilities from existing biogeochemical reaction models. Another key capability is Amanzi-ATS's flexibility in handling multiple computational meshes and process models, which has enabled a novel multiscale model structure [4] that makes it possible to represent biogeochemical process understanding gained from laboratory or small-scale field investigations in much larger models. Watershed-scale reactive transport simulations for Copper Creek Watershed, East River, Colorado demonstrate the fully coupled integrated hydrology RTM capability, and network-scale simulations of nutrient dynamics in the Portage River Basin, Ohio demonstrate the multiscale capability. This work emphasizes the need for flexible modeling frameworks that allow for deployment of new capabilities while supporting the implementation of complementary approaches.

[1] Coon, E. et al. "Advanced Terrestrial Simulator." Computer software. September 10, 2019. https://github.com/amanzi/ats. https://doi.org/10.11578/dc.20190911.1.

[2] Molins et al., A new approach to simulate integrated-hydrology and reactive-transport modeling, In preparation.

[3] Molins et al., Alquimia: A generic interface to biogeochemical codes– A tool for interoperable development and benchmarking, In preparation.

[4] Jan, A., Coon, E.T., Painter, S.L. 2021. “Toward more mechanistic representations of biogeochemical processes in river networks: Implementation and demonstration of a multiscale model”, In Review.