High Performance Computing for Understanding Aggregate C-Q Relationships in Watersheds

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Abstract:

The Concentration-Discharge (C-Q) relationship is widely used as a measure of the dynamics of the relevant processes across the different watershed systems and hydrological compartments. Understanding how watershed compartments interact with one another to produce the observed C-Q data is crucial to predict how perturbations, such as drought and its consequences on surface water-groundwater interactions, affect the hydrogeochemical response.

In this work, we used high-performance computing tools to understand the impacts of integrated surface-subsurface flow driven by evolving climate drivers on weathering reactions and thus on chemical exports. In partnership with IDEAS-Watersheds, we implemented reactive transport processes in the Advanced Terrestrial Simulator (ATS) using a flexible multiphysics framework (Molins et al., submitted). The integrated reactive transport process kernel (PK) was weakly coupled to integrated hydrology PK, and integrated transport and reactions were coupled using an operator splitting approach.

The new capabilities were used to simulate integrated hydrology and reactive transport in the Copper Creek catchment (Xu et al., submitted). A 3D 50-m-resolution model was constructed to simulate a 10-year period (2010-2019) using NERSC supercomputers. The model captured the distinct hydrogeochemical responses observed in the average (WY16), wet (WY17) and dry (WY18) years, and was used to quantify the groundwater and surface water mixing in the form of C-Q relationships. Modeled C-Q relationships suggested that pyrite dissolution was affected by the changing hydrological drivers where it was enhanced in the dry year. When shallow water dominated stream discharge under high flow conditions, calcite dissolution supplemented calcium dilution. Spatially-resolved results showed higher soil saturation and snowpack declines occurred

earlier across the south-facing slopes relative to the north-facing. This is a first-of-its-kind demonstration of high-resolution modeling to enable predictive understanding of hydrogeochemical exports in response to climate and other disturbances affecting surface-subsurface dynamics.

Current efforts have shifted to developing a comprehensive integrated reactive transport model of the Lower Triangle region to understand the processes affecting nitrogen exports. Integrated hydrology results show that changing surface-subsurface interactions trigger different flow regimes and runoff generation mechanisms, hence affecting the distributed hydrological response (Ozgen-Xian et al, submitted). These findings suggest that distributed hydrological responses may not be reflected through aggregated hydrological signatures. Using remote sensing and survey data, integrated through machine learning, we parameterize spatially-distributed land cover, soil thickness, geological and geochemical properties. The reactive transport model is being used to estimate nitrogen exports linked to changes in the hydrological cycle in this mountainous watershed.

Molins, S., Svyatsky D., Xu, Z., Coon, E.T., Moulton, J.D., A multicomponent reactive transport model for integrated surface-subsurface hydrology problems, submitted to Water Resources Research.

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Ozgen-Xian, I., Molins, S., Johnson, R.M, Loritz, R., Xu, Z., Dwivedi, D., Mital, U, Ulrich, C, Steefel, C.I., The role of surface–subsurface interactions in the distributed hydrological response of a headwater-dominated catchment, *in review* Hydrological Processes.