The Watershed Function SFA: Mountainous System Hydrobiogeochemical Response to Disturbance across Genome to Watershed Scales

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Abstract: Uncertainty associated with predicting watershed hydrobiogeochemical behavior remains high as climate change, wildfire, land-use change, and other disturbances significantly reshape interactions within the world's watersheds. The Watershed Function SFA ("SFA") is reducing this uncertainty through advancing a predictive understanding of how **mountainous watersheds retain and release water, nutrients, carbon, and metals, particularly in response to snow dynamics and disturbances such as droughts, floods and wildfire.** The project is being undertaken at the mountainous headwater East River Watershed of the Upper Colorado River Basin. Streamflow originating from snowpack in this Basin provides the majority contribution to the Colorado River, which is critical for Western U.S communities, energy, agriculture, and industry.

The responses of mountainous systems to disturbance are particularly complex, involving multi-physics, multi-scale processes occurring from bedrock through canopy, across land-water interfaces, from genome-to-watershed scales and across extreme lateral gradients in elevation, vegetation and geology. To tractably confront this complexity, the SFA is developing new ways of conceptualizing, characterizing and predicting aggregated watershed system behavior. In particular, the SFA takes a system-of-systems approach, using remotely sensed and other information to identify key watershed subsystems or "functional zones". These zones are hypothesized to have unique properties (relative to neighboring parcels) that influence that zone's response to disturbance. To test the SFA functional zone concept, observations, experiments and modeling are performed within distinct, archetypal parcels to provide insights about how zones uniquely respond to snow dynamics. This information is in turn used to inform larger-scale predictions of aggregated, time-variable watershed concentration-discharge signature, using scale-adaptive watershed simulation (SAWaSC) and functional zone modeling capabilities. The SFA current phase focuses on developing a predictive understanding of aggregated water and nitrogen exports in response to snow dynamics.

The Watershed Function SFA has realized significant progress during this reporting period, leading to 54 papers that are published or in review. Select examples of progress this year include:

- Quantification of precipitation partitioning as a function of season and watershed characteristics and documentation that monsoons are not likely to compensate for decreased snowmelt in terms of streamflow generation;
- Deep quantification of the East River microbiome and how it varies with vegetation type, river meander and hillslope characteristics, and snowmelt dynamics;
- Quantification of the role and magnitude of bedrock weathering on watershed nitrogen exports and the first watershed-wide simulation of nitrogen cycling and exports;
- Developed and successfully tested a watershed zonation construct, finding that the extreme watershed heterogeneity could be accurately and tractably represented using just six zones;
- Acquired and archived a staggering diversity and volume of data from the East River site, which now includes >600 physical sensors, >100 million data points, and >100 data types.

Reconciling Evapotranspiration – Cross Method Synthesis, Uncertainty Quantification, and Path Forward

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Abstract: Accurate quantification of evapotranspiration (ET) is a common and fundamental challenge in predicting watershed hydrological behaviors. Large ET uncertainties stem from a multitude of sources depending on method-of-choice and scale. Two major factors are contributing to ET uncertainties and the difficulties in reconciling discrepancies among different methods, namely (a) unknown true ET values, and (b) differences in meteorological inputs and ET formulations. Understanding sources of uncertainty and developing gold-standard benchmarking platforms and datasets are key to accurately predicting ET rates and drivers at watershed scales and beyond.

We summarize recent progresses of the Watershed Function SFA on these challenges, highlighting (a) development of ET benchmarking platforms and datasets, and (b) reconciliation of various ET methods used at East River to identify sources of uncertainties. Combining these efforts will lead to significant improvements of ET quantification from local to watershed scales at the East River and beyond.

Specifically, gold-standard, best-in-practice methods were established at both the laboratory and field scales to for ET benchmarking. These include the lysimeter style SMARTSoils testbed at the Berkeley lab, and Eddy Covariance/Energy Balance systems, flux tent, water mass-balance, and sap-flow datasets in the field. The reconciliation efforts explored a multitude of ET methods, ranging from physics rich Penman Monteith model to petrophysics style models such as Priestley-Taylor, and across spatiotemporal scales from sub-minute to year-around meter scales at intensive sensing sites to multi-decadal studies across the East River watershed. We also included a wide range of methodologies ranging from stand-alone ET formulations to comprehensive modeling platforms, to isotopes.

While ET estimates vary significantly among different methods, there is consensus regarding transitions between water and energy limited systems across locations and years, and the need to understand the differing mechanistic drivers and responses for evaporation (E) and transpiration (T) across functional zones. Further, all methods point to the lack of true ET datasets for model

parameterization and benchmarking, and the inconsistency and insufficiency of meteorological and soil/plant measurements in resolution and scales, both of which calls for the consistent use of high-quality datasets across all methods. Continuing efforts will focus on the alignment of different methods on a common set of benchmarking locations, such as the pumphouse hillslope and Snodgrass intensive sites, and the collection and utilization of gold-standard datasets discussed above for model validation and improvements, which include the upcoming SAIL campaign that produces high quality meteorological data.

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Chen, J., B. Dafflon, A. P. Tran, N. Falco, and S. S. Hubbard (submitted), A Deep-Learning Hybrid-Predictive-Modeling Approach for Estimating Evapotranspiration and Ecosystem Respiration, Hydrology and Earth System Sciences, DOI: 10.5194/hess-2020-322.

Ryken, A., Gochis, D., Maxwell, R. Unraveling groundwater contributions to evapotranspiration in a mountain headwaters: Using eddy covariance to constrain water and energy fluxes in the East River Catchment. Submitted to Hydrological processes. DOI: 10.22541/au.160974909.94645181/v1

Snowmelt Dynamics and its Contributions to Catchment Water Partitioning

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Abstract: We describe investigations combining observations and simulations of hydrometric (precipitation, discharge, snowpack) and stable isotope (^{2}H &^{18}O) data to infer the role of snowmelt in discharge generation in Colorado's East River Watershed. The first investigation assesses mechanisms of snowpack isotopic loading into the soil and the impact on recharge dynamics using PRMS coupled to a new snow isotope fractionation model (Carroll et al., in review). The latter was calibrated to observed spatiotemporal variability of snowpack volume and isotopes. We found that seasonal variability and elevation primarily control volume and isotopes of influx, and that snowpack isotopic fractionation via evaporation and melt account for only <5% of the influx variability. Our modelling indicates that recharge is highest in the upper subalpine. The simulated isotopes in this zone match groundwater observations, providing evidence that the upper subalpine is a preferential recharge zone in mountain systems.

In a second investigation, we infer rain vs. snow contributions to evapotranspiration and summer discharge using isotope mass balance approaches in seven East River subcatchments. The results confirm that snow dominates evapotranspiration and summer discharge (ca. 80%). About 50% of rainfall evapotranspired and <20% became summer discharge. Tree density best explains inter-catchment variability, as subcatchments with higher tree density have a larger share of evapotranspiration sourced by rain, more rain evapotranspiring, and less rain sustaining summer discharge. These findings agree with recent PRMS simulations showing monsoon rain cannot replenish water deficiency from lower snowpack (Carroll et al., 2020).

Particle tracking from an integrated hydrologic model (ParFlow-CLM-EcoSLIM) shows agreement with the isotope mass balance for ET fraction from snow across subcatchments. However, the two methods have differences in evapotranspiration sums, driving substantial mismatch in the fraction of snow evapotranspired. Future work will reconcile these differences by determining the effects on mass balance of groundwater storage changes and uncertainties in precipitation forcing.

To better assess the variability in snowpack thickness, snowmelt timing, and soil freeze-thaw intensity, we deployed a sensor network of a Distributed Temperature Profiling system developed at Berkeley Lab across 30 locations monitoring soil and snow temperature with unprecedented spatiotemporal resolution. The measurements indicate strong impacts of slope and aspect on the

snowpack dynamic, with South-West facing slopes without soil freezing and first bare-ground date up to one month earlier than the North-East facing slopes.

These approaches shed critical light on the timing and volume of snowmelt as a driver for heterogeneous hydrological responses in mountainous watersheds.

Carroll, R.W.H., Gochis, D., Williams, K.H., 2020. Efficiency of the summer monsoon in generating stream flow within a snow-dominated headwater basin of the Colorado River. Geophys. Res. Lett. 47, doi10.1029/2020GL090856

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Leveraging Genomes for Quantitative Insights into Microbiome Influence on Watershed Function – a synthesis from the Watershed SFA at East River, CO

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Abstract: Scaling microbiome processes to watershed or basin scales is a challenge due to the fine scale at which microbes interact with their environment. An open research question in watershed science is to what extent microbiome properties affect aggregated watershed functions? The Watershed Function SFA, aims to develop a predictive understanding of aggregated watershed responses to perturbations. We hypothesize that the spatial distribution of microbial functional traits can improve predictions of aggregated watershed function in space and time. We are testing this hypothesis through 1) strategic field sampling of metagenomes in key watershed locations during critical periods of the hydrologic cycle (e.g., snowmelt or baseflow), 2) targeted lab experiments to discover the diagnostic microbial metabolic pathways responsible for nutrient retention versus loss, 3) use of metabolomics and genome-inferred traits to parameterize reactive transport models. To facilitate this watershed scale synthesis, we are constructing an interoperable and reusable resource for all microbial multi-omic, microbial trait, and soil biogeochemical data collected from East River.

Across seven synergistic campaigns microbial processes have been interrogated along a continuum from bedrock to canopy, focused on key watershed domains including upland hillslopes, multiple meanders along the river corridor, and at mineral weathering interfaces in the subsurface or the rhizosphere. Topographic position in the landscape, vegetation type, and snowpack properties all shape microbiome features, although we have observed remarkable consistency in genome and functional trait frequency in specific watershed domains. An intensive field campaign was carried out, where 400 samples were obtained from 13 locations across four catchments in the upper East River watershed varying in elevation, hydrological and geological properties, and dominant vegetation types. This was concurrent with an NSF NEON Airborne Observatory Platform imaging flight (hyperspectral and LiDAR) over the study area. In partnership with the JGI, we have obtained 724 metagenome samples, completed assemblies from 511 and binning of 371, together comprising at least 91K microbial species. We are currently synthesizing these observations, using genome-inferred traits to define microbial functional guilds and their watershed scale distributions. Integration of airborne remote sensing surveys (geomorphology, snowpack and vegetation distributions), plus advanced geophysical sensing allows quantification of co-variance between microbiomes, soil biogeochemistry and surface observable properties. This information allows us to parameterize genome-informed reaction networks and their microbial

kinetics, and using machine learning approaches, to derive suites of surface observables properties that are predictive of microbial functional trait and genome distributions across the watershed.

Lavy, A., McGrath, D. G., Matheus Carnevali, P. B., Wan, J., Dong, W., Tokunaga, T. K., ... & Banfield, J. F. (2019). Microbial communities across a hillslope-riparian transect shaped by proximity to the stream, groundwater table, and weathered bedrock. Ecology and evolution, 9(12), 6869-6900.

Carnevali, P.B.M., Lavy, A., Thomas, A.D., Crits-Christoph, A., Diamond, S., Méheust, R., Olm, M.R., Sharrar, A., Lei, S., Dong, W. and Falco, N., 2021. Meanders as a scaling motif for understanding of floodplain soil microbiome and biogeochemical potential at the watershed scale. Microbiome, 9(1), pp.1-23.

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Bedrock–Watershed Connections and Conundrums

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Abstract: Bedrock stores and releases water, nutrients and chemical energy on a large range of timescales. Sedimentary rock, for example, can preserve for millions of years organic molecules generated by ancient biological carbon and nitrogen fixation, and reactive minerals precipitated through biogeochemical processes. Uplift and exposure of bedrock initiates chemical and biological weathering that mobilizes these elements into groundwater and back into terrestrial biogeochemical cycles. On the seasonal-to-decadal timescale, fractured and porous bedrock can transiently store water, organic and inorganic carbon, and other redox-active elements as precipitation patterns and groundwater transport vary. The ecological impacts of bedrock in mountainous watersheds, which are often water- and nutrient-limited, and which experience relatively fast rates of weathering, can be particularly important but remain poorly quantified.

The Watershed Function SFA, located in the snow-dominated mountainous headwaters of the East River, CO, and surrounding catchments, is revealing the roles for bedrock as a reservoir of water and elements. Groundwater and subsurface gas measurements have shown that the weathering of organic-rich marine shale can be a significant source of biologically available nitrogen (*Wan et al.,* 2021). High-resolution imaging of the records of rock weathering have established the geochemical reaction networks controlling the release of elements to groundwater (*Lavy et al.,* 2019). Distributed metagenomic studies have connected rock-derived elements to microbial metabolism and found that proximity underlying Mancos shale apparently controls species distribution (*Carrero Romero et al.*, in prep). Watershed-scale geophysical and remote sensing are establishing how bedrock composition (e.g., types, hydrothermal alteration), topography and subsurface structure influence vegetation distribution and susceptibility to drought. Soil-to-bedrock vegetation harvesting discovered deep roots of perennial shrubs to penetrate to regions of weathering bedrock, suggesting a strategy for acquisition of water or nutrients. High-frequency stream water measurements uncovered distinctive trace-element patterns likely caused by motions on the faults or fractures connecting from subsurface rocks to the watershed.

These findings demonstrate multiple ways in which bedrock and surficial processes are connected, but questions and challenges remain. In particular, the ecohydrogeological factors that determine the biogeochemical retention, cycling or export of bedrock derived elements remain to be

established and quantitatively scaled across this geomorphologically diverse landscape. Although measurement and modeling of the trends in chemical composition of the East River and its tributaries can distinguish impacts of watershed processes (*Arora et al.,* 2020), understanding the temporal and climate feedbacks between rock, plant and microbial processes that control water and element retention or loss remains an ongoing objective addressed through new studies in and around this catchment.

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Towards a Conceptual Framework of Watershed Nitrogen Retention and Loss across Scales

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Abstract: Patterns of watershed nitrogen (N) retention and loss are shaped by how watershed mechanistic processes retain, biogeochemically transform, and lose incoming atmospheric and geogenic sources of N. Recent studies in snowmelt-dominated catchments have documented changes in nitrogen (N) retention over time, such as declines in watershed exports of N (*Newcomer et al.,* 2021), though a comprehensive framework accounting for process-based interactions operating at different spatial and temporal scales is still missing. Synthesizing experimental and modeling N-studies in the East River, we assess application of the novel Watershed Index for Retention and Loss (WIRL) concept as it relates to N.

Our synthesis aggregates local-to-basin scales using 1500 datapoints of concentration-discharge (C-Q) signals, subsurface/surface/soil/plant sampling across different compartments and ecoregions, paired-catchment analysis, and subsurface and surface modeling down the river corridor. The WIRL concept suggests that functional information about the landscape (retention and loss) can be found within signals that aggregate those mechanisms. C-Q signals in the river corridor are one such example of a signal that aggregates information from the landscape. An examination of differential C-Q signals at three main East River sites, each near floodplain riparian zones, suggest the meandering downstream section is marked by gains in both groundwater and NO_3^- concentrations as opposed to the dilution and the declining trends observed in the high-relief, steep terrain upstream reach (*Arora et al.,* 2020). Modeling work at the local and watershed scales help to narrow the range of mechanisms controlling the observed C-Q trends. At the local scale, modeling of floodplain riparian hollows suggest they functionally act as inhibitors to upland hillslope NO_3^- reaching the stream (35-55% removed) (*Rogers et al.,* 2021). At the watershed scale, we developed the High-Altitude Nitrogen Suite of Models (HAN-SoMo), a watershed-scale ensemble of process-based models of the East River Watershed (*Maavara et al.,* 2021). While geogenic sources account for approximately 12% of the annual dissolved N sources to the watershed, on an annual scale, instream dissolved N elimination, plant turnover (including cattle grazing) and atmospheric deposition are the most important controls on N cycling. These studies reveal that retention of N in subsystems of the watershed is highly heterogeneous and a potential function of presence or absence of floodplains, plant dynamics, and highlights the importance of

transformations once N reaches the stream. At the watershed and basin scale we validate the first application of the WIRL concept at an unprecedented scale across the CONUS that links instream nitrogen signals to upstream mechanistic landscape processes (*Newcomer et al.,* 2021).

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Advanced bedrock characterization of a mountainous watershed using geological and geophysical data, and machine learning

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Abstract: Bedrock properties are critical for understanding and predicting the hydrological response of watersheds to climate disturbances. Estimating these properties on a watershed-scale is inherently difficult, particularly for fractured-bedrock dominated domains. Our analysis provides the first study to test the co-variability of above and below ground features on a watershed-scale, based on extensive airborne electromagnetic (AEM) data, surface and borehole geophysical data, and high-resolution remote sensing data. We use machine learning approaches to quantify the relationships between bedrock geophysical/hydrological properties and geomorphological/vegetation indices at the East River Watershed, CO, and show that these relationships can be used to estimate the first order variability of bedrock properties throughout the watershed. By assessing the stationarity of these relationships, we show that regions of smaller variability in the input parameters, i.e. slope, aspect, elevation, and vegetation cover, provide more accurate estimates of bedrock properties, highlighting the limitation of commonly applied geomorphological models that rely solely on above-/below-ground co-variability.

Through this analysis we identified previously unmapped fracture zones. To identify the origin of one such fracture zone, we developed a Popper-Bayes hypothesis testing method that incorporates machine learning elements. Based on this approach, we falsified several geological models, and concluded that the most likely origin of this fracture zone, which is crossing one of the Watershed intensive sites, is either a normal or high-angle reverse fault, or a potential sackung feature. This result implies that auxiliary features associated with the fracture zone, such as offset geological layers, may also be present in the watershed.

Combining these detailed studies of bedrock properties with state-of-the-art geological modelling approaches, we have developed a 3D geological model of the entire East River Watershed and beyond. This model, integrating various bedrock characterization approaches, is building the basis for novel flow and transport modelling tasks and targeted subsurface property investigations. These studies highlight that a multi-scale characterization of a watershed from plot to regional scale, as we performed, is required to enable detailed modelling of subsurface flow and transport to assess the impact of disturbances onto such hydrological systems.

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Watershed zonation approach for tractably quantifying above-and-belowground watershed heterogeneity and functions

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Abstract: Predictive understanding of watershed functions is often hindered by the heterogeneous and multiscale fabric of watersheds. In this study, we have developed a watershed zonation approach for characterizing watershed organization and functions in a tractable manner by integrating multiple spatial data and model output layers. Recognizing the coupled ecohydrogeological-biogeochemical interactions that occur across bedrock through canopy compartments of a watershed, we hypothesize that (1) suites of above/belowground properties co-varying with each other, (2) machine learning methods can be used to identify watershed zones having unique distributions of bedrock-through-canopy properties relative to neighboring parcels, and (3) property suites associated with the identified zones can be used to understand zone-based functions, such as response to early snowmelt or drought, evapotranspiration, and associated solute exports to the river. This zonation approach essentially reduces the complexity or multidimensionality of watershed heterogeneity into a set of zones.

We have explored multiple zonation constructs to capture multiscale natures of heterogeneity as well as various watershed patterns and functions – based on both observations and modeling results – at the East River Watershed near Crested Butte, CO. We first developed unsupervised clustering methods that synthesizes airborne remote sensing data (LiDAR, hyperspectral, and electromagnetic surveys) and bedrock-to-canopy co-variability. Using independently collected data, it is shown that the identified zones capture the heterogeneity of key watershed functions at the watershed scale, including foresummer drought sensitivity and river nitrogen exports. Second, we have applied unsupervised clustering to the input and output data layers of a watershed-scale integrated hydrological model, which found the co-variability of elevation and topographic metrics and key hydrological functions such as water table dynamics and evapotranspiration. In addition, at the hillslope scale, we have developed a zonation approach that captures plant dynamics time-series and soil moisture associated with microtopography. These results combined have contributed significantly to selecting hillslope experiment locations as well as optimizing a large-scale monitoring network of snow, precipitation, and soil moisture.

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Multiscale Analysis of Watershed Function with High Resolution Process-Based Models

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Abstract: We are using high-resolution process-based modeling to quantify aggregated water and biogeochemical cycling at the watershed scale. This modeling is carried out at multiple scales, beginning with individual soil pits and boreholes, extending to 2D hillslope and floodplain transects, 3D hillslope, and 3D sub-catchment scale, and combines both high-resolution surface-subsurface water modeling with reactive transport. Our ultimate objective is to quantify solute and nutrient export (especially nitrogen) to the stream network in the East River watershed, considering flow, bedrock weathering, and shallow soil and vegetation processes, all within the context of transient climate forcing and other disturbances.

This research component includes:

- *Zone-based transect modeling:* Functional zones have been identified that depend in part on the distinctive characteristics of the hillslopes. For each functional zone, we are creating a hillslope scale model (typically in 2D) to examine hillslope and floodplain connectivity that impacts river chemistry and comparing its response to early snowmelt. The analysis is also being extended to consider deep time weathering of bedrock to determine how this influences present day and future chemical export to the stream network.
- *Reduced dimension 1D modeling of flowtubes to represent hillslope fluxes:* With the development of a new computationally efficient approach to modeling transient flow and reactive transport in flowtubes, we are quantifying the aggregated hillslope fluxes to the stream network.
- *3D HPC modeling of surface+subsurface flow and biogeochemistry:* Using the software platform Amanzi-ATS, we are developing models for flow and biogeochemistry at the sub-catchment scale, initially focusing on the Copper Creek and the Lower Triangle. These computationally-intensive simulations provide direct predictions of C-Q responses in the East River system, while capturing the spatially-distributed processes that underpin these responses using multi-resolution meshes. They also provide synthetic data for machine-learning based reduced order models.
- *SAWASC: Functional Zone-based reduced-order modeling to predict Aggregated Watershed discharge and nitrogen export:* Building on insights from the HPC modeling task, a reduced-order SAWaSC (Scale Adaptive Watershed Simulation Capability) modeling approach is being developed to predict aggregated watershed discharge and nitrogen as a function of snow dynamics. The approach is based on a residence time analysis within stretches of the river system, with lateral bedrock and hyporheic exchange taken from *machine learning-based training* on the high resolution distributed HPC sub-catchment simulations of biogeochemical

cycling and fluxes. The zonation will be used to provide time-dependent lateral fluxes of water and biogeochemical species to the river system, i.e., C-Q relationships.

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