ANNUAL REPORT

Watershed Function Scientific Focus Area (SFA)

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watershed.lbl.gov

Watershed Function SFA:

Biogeochemical Dynamics from Genomes to Watershed Scales

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1.0 WATERSHED FUNCTION SFA OVERVIEW

Increasing human populations and resource-intensive lifestyles drive a growing demand for clean water, food, and energy. While society is critically dependent upon water resources and the biogeochemical benefits provided by watersheds, the scientific community is at an early stage of developing a predictive understanding of how watersheds function as integrated hydro-biogeochemical systems, and how these systems respond to perturbations, such as those caused by changes in weather, land use, vegetation cover, snowmelt timing, and contaminant loading. Recognizing the societal importance yet vulnerability of mountainous watersheds to such perturbations, the Watershed Function SFA poses **an overarching question of 'how do perturbations to mountainous watersheds, such as droughts, floods or early snowmelt, impact downstream water, nutrient, carbon, and metal release?'** This project focuses on improving predictions of mountainous watershed dynamics at **episodic and seasonal to decadal** timescales, where scientific foundations are needed to inform optimal resource management. The watershed function expertise and capabilities developed through this project are expected to provide a critical underpinning for many energy and environmental challenges, including: contaminant mobility, nutrient delivery for sustainable biofuel crops, reliable and clean water delivery, and sustainable water and hydropower resources.

Several formidable challenges inhibit a predictive understanding of watershed function and dynamics across length and time scales relevant for resource management. Examples include the wide variety of complex interactions that occur in a watershed between plants, microorganisms, organic matter, minerals, dissolved constituents, and migrating fluids, and the wide range of scales and heterogeneous watershed compartments within which these interactions occur. Particularly challenging is the quantification and prediction of how coupled hydrologic, vegetation, and biogeochemical interactions, which occur from bedrock-through-canopy, respond to perturbations in complex domains. These interactions vary as a function of elevation and landscape location, with different and often localized responses to earlier snowmelt, increasing temperatures, and other perturbations. Quantifying the spatial variability of the coupled responses to perturbations, and how responses propagate throughout the system and generate an integrated watershed discharge response, constitute a major scientific challenge.

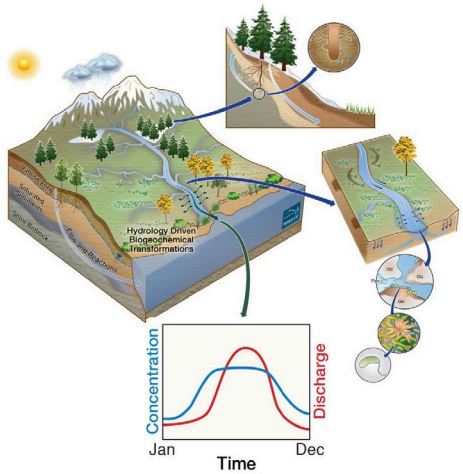


Figure 1. The Watershed Function SFA takes a system-within-system perspective and is using a scale-adaptive approach to quantify how spatially variable responses to perturbations propagate through the system and lead to an aggregated downgradient watershed discharge and concentration signature.

The Watershed Function Scientific Focus Area (SFA) is advancing a predictive understanding of watershed function and dynamics through explicit consideration of the scientific challenges defined above. The project is guided by several constructs. First, the Watershed Function SFA take a holistic perspective of the watershed, considering the integrated role of surface and subsurface water flow, mass transport, and biogeochemical reactions – from bedrock to the top of the vegetative canopy, from terrestrial through aquatic compartments, and from summits to receiving waters (Fig. 1). The Watershed Function SFA has developed a system-of-systems perspective, based on consideration of archetypal subsystems within the watershed and their aggregation to yield a cumulative discharge-concentration signature (Fig. 1). A 'scale-adaptive' construct serves as the organizing framework for the SFA. Herein, we define scale-adaptive as characterization, simulation, and data science approaches that explicitly confront the hierarchical nature of watershed systems for improved predictive understanding. Scale-aware characterization approaches include the development of nested and networked sensing systems, ultimately providing minimal but sufficient distributed information to diagnose of watershed responses to perturbations. Scale-aware simulation capabilities include adaptive mesh refinement (which can resolve finer scale features and behavior relative to neighboring regions) and

adaptive modeling (wherein differing physics and mathematical algorithms may be used at different scales). Building upon the genome-enabled watershed simulation capability that was successfully developed and tested up to the floodplain scale during the previous phase of this SFA at Rifle CO, and pointed at increasing computational resources expected to be available as part of the exascale trajectory, the first-ever watershed scale-adaptive simulation approach is intended to permit simulation of system-within-systems behavior – and aggregation of that behavior – up to the watershed scale.

The Watershed Function SFA focuses on mountainous watersheds due to their societal importance, complexity, and vulnerability to environmental change. Observational evidence suggests that mountain water resources and associated services important for society are being threatened by global warming trends (e.g., Beniston and Stoffel, 2014). Climate change has already begun to affect mountain systems in the past few decades by altering snowpack and snowmelt timing (e.g., Lukas et al., 2015). These changes are attributed to increased temperatures, causing transitions in precipitation from snowfall to rainfall, which results in a delay of snowpack accumulation in the fall and throughout the remainder of the snow season. Decreased snowpack results in lower albedo, increasing the surface absorption of solar radiation. Greater absorbance of short- and longwave radiation serves to increase soil temperature and decrease soil moisture (Fyfe and Flato, 1999; Rangwala et al., 2013; I T Stewart et al., 2005; Stewart, 2009), which, along with increasing air temperature, can contribute to vegetation mortality and vegetation succession in mountainous systems (Allen et al., 2010; A P Williams et al., 2013). This combination of climate and vegetation drivers non-uniformly alters the distribution of evapotranspiration patterns at the scale of the watershed, leading to earlier snowmelt, shifting patterns of soil water utilization, decreased streamflow and groundwater recharge, increased fluid residence times (Engdahl and Maxwell, 2015), and increased metals loading (Manning et al., 2013; Todd et al., 2012). These changes have largely unknown impacts on biogeochemical interactions, including those associated with plant-soil microbial processes and microbe-mineral dynamics (Bearup et al., 2014; Mikkelson et al., 2013).

The Watershed Function SFA is being carried out within the East River watershed in the Upper Colorado River Basin, a region that constitutes a study domain of ~300 km^2, including both pristine and metals-impacted drainages. The watershed encompasses gradients in elevation and life zones from uplands to hillslopes to floodplains to downgradient receiving surface waters. We have developed a number of intensive and satellite sites in different subsystems of the watershed (Fig. 2), which were chosen to represent regions having distinct couplings and responses to perturbations. The Watershed SFA science questions are being addressed by investigating and extrapolating the subsystem intensive site response functions and observations to the watershed scale using remote sensing and other datasets tightly coupled to models. While we are developing the SFA system-of-systems and scale-adaptive approaches at East River, given the importance of mountainous watersheds to mankind, we expect that insights and capabilities developed as part of this SFA will have potential for both national and worldwide impact.

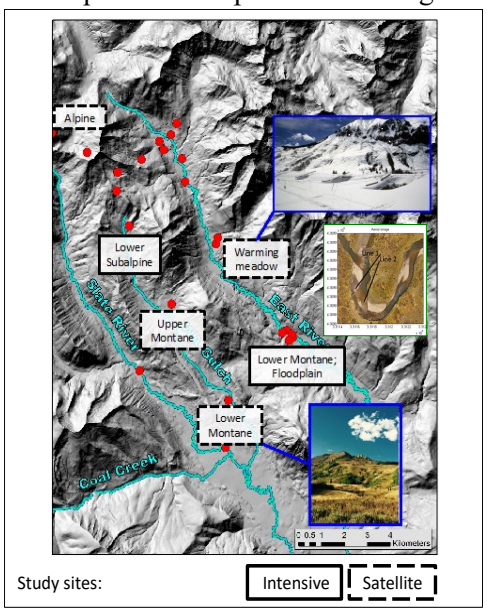


Figure 2. The 300 km^2 East River Watershed SFA science questions are being tackled through investigation at and between a suite of intensive and satellite sites, each expected to have distinct coupled vegetation-hydrology-biogeochemical responses to perturbations.

Developing approaches to accurately predict watershed function and dynamics is directly aligned with the BER-CESD mission to provide the fundamental science needed to inform the development and deployment of advanced solutions to the Nation's energy challenges, including enhancing the seasonal to multi-decadal predictability of the Earth system using long term field experiments, DOE user facilities, modeling and simulation, uncertainty characterization, best-in-class computing, process research, and data analytics. Of the five Grand Challenges identified in the 2018 CESD Strategic Plan, the Watershed SFA is particularly well aligned with the

'Integrated Water Cycle', 'Biogeochemistry' and 'Data-Model Integration' Challenges. It is also very well aligned with the BER-SBR overarching objective to advance a robust predictive understanding of how watersheds function as integrated hydro-biogeochemical systems, and how these systems respond to perturbations. Meeting this objective requires transformational advances in our ability to quantify and predict the mechanisms by which hydrology drives fine scale biogeochemical processes in surface-subsurface systems, and to translate key information across relevant molecular to watershed scales.

2.0 SCIENTIFIC QUESTIONS AND MILESTONES

The Watershed SFA is driven by a single Grand Challenge, which is being tackled through addressing six supporting science questions.

Grand Challenge:
How do mountainous watersheds retain and release water, nutrients, carbon and metals?
How will droughts, early snowmelt and other perturbations impact downstream water availability and biogeochemical cycling at episodic to decadal timescales?

SFA Supporting Science Questions.

Question 1: How do perturbations to individual watershed subsystems, including early snowmelt and drought, lead to changes in downgradient export of water, N, C & P from that subsystem?

Question 2: How do early snowmelt and/or droughts alter subsystem connectivity and fluid residence times within mountainous watersheds, including bedrock?

Question 3: How do interactions between vegetation, hydrology, subsurface biogeochemistry and geology, particularly in response to perturbations, vary along diverse watershed gradients (vegetation, hydrogeology, elevation, redox) and contribute to aggregated N, C, P and trace metal exports from the watershed?

Question 4: When and where does fine-scale representation of processes significantly improve prediction of watershed nutrient dynamics, and how can those processes be tractably represented in mechanistic watershed models?

Question 5: Do perturbations that impact water flow and nutrient transport in pristine systems enhance or suppress metals release from mining-impacted systems having otherwise similar watershed characteristics?

Question 6: Which insights and methods are critical for improving operational forecasting predictions of water quantity in response to a range of pulse and press perturbations?

The supporting science questions build upon each other, spanning from individual subsystems (Question 1) to aggregated watershed response (Question 3), and using the developed insights to address inherently challenging fundamental scaling questions related to the influence of small scale processes (Question 4) and the impact on larger basin scale operational forecasting (Question 6). Question 5 expands the SFA early work in the pristine part of the East River catchment to a metals-impacted region. Each of the Supporting Science Questions is carried out through a series of tasks, collectively involving multi-disciplinary expertise and data-model integration. To measure success, each Supporting Science Question has well-defined three, six and nine-year milestones.

For the FY17-FY19 phase of the Watershed Function SFA, we focus primarily on Questions 1-3, which are explored in the pristine region of the watershed, with complementary tasks underway with DOE-funded University and USGS collaborators to enable out-year progress on Questions 4-6. In this limited-page Annual Report, we correspondingly focus primarily on describing task accomplishments associated with Questions 1 and 3. Given the importance of snowpack and snowmelt timing to exports from mountainous systems, we focus in this early stage on responses to snowmelt. Over the period of study, the site has been subject to a wide range of snowpack and snowmelt timing conditions (Fig. 3), providing a natural laboratory with which to test our approaches. The SFA has also identified crosscutting milestones important for addressing the Grand Challenge question. The crosscutting milestones build upon and integrate across advances made through tackling the Supporting Science Questions. The overarching SFA three-year milestone was carefully chosen to: (a) enable tractability over a three-year time period, (b) foster integration

across science theme teams and supporting science questions toward a common goal, (c) exercise the newly developed scale-aware simulation capabilities, and (d) address a key subset of our overarching question.

SFA Three-Year Overarching Milestone:
Evaluate the hydrological controls on the sources and sinks of nitrogen across a mountainous watershed composed of heterogeneous hotspots and use scale-adaptive approaches to represent the feedback between hydrological perturbation and above- and below-ground biogeochemical processes to improve predictions of nitrogen export from the catchment.

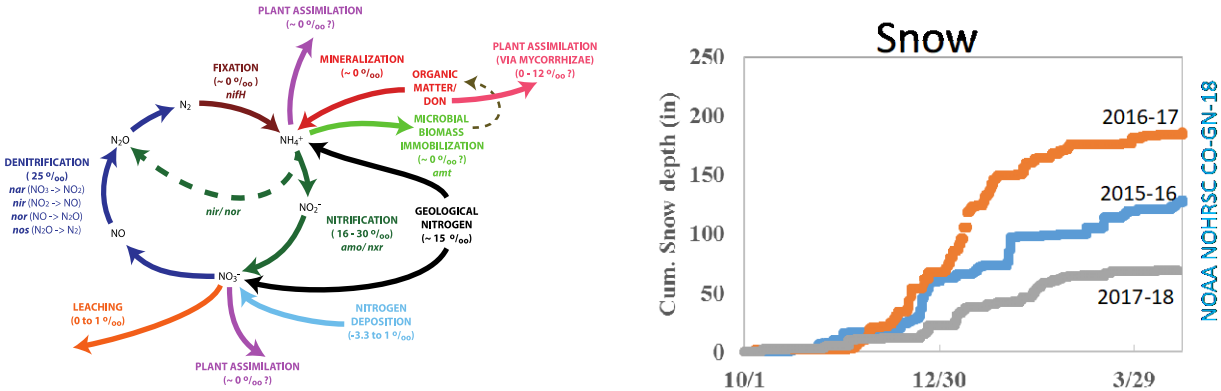


Figure 3. The early phase of the SFA focuses on testing scale-aware approaches to understand the aggregated nitrogen exports and the responses of the system to variations in snowmelt timing. The right figure indicates that the site has been subject to low, high and normal snowmelt accumulation with variable snowmelt timing over the last few years, providing a fortuitous set of natural conditions with to test our approaches.

3 ORGANIZATION

The SFA team includes ~70 individuals distributed across Berkeley Lab, five universities, government, and private sector companies. The project is composed of six components representing the scientific themes of the project. The SFA organizational structure facilitates two aspects, which are important for project success: (a) investigations of specific hypotheses associated with scientific themes (hydrology, ecohydrology, and organomineral dynamics); and (b) integration of multiple component expertise to tackle the six supporting science questions described above. The project and component leads (Fig. 4) along with Harry Beller and Jill Banfield comprise the Watershed Function executive committee. Component task leads, including many early career staff, are

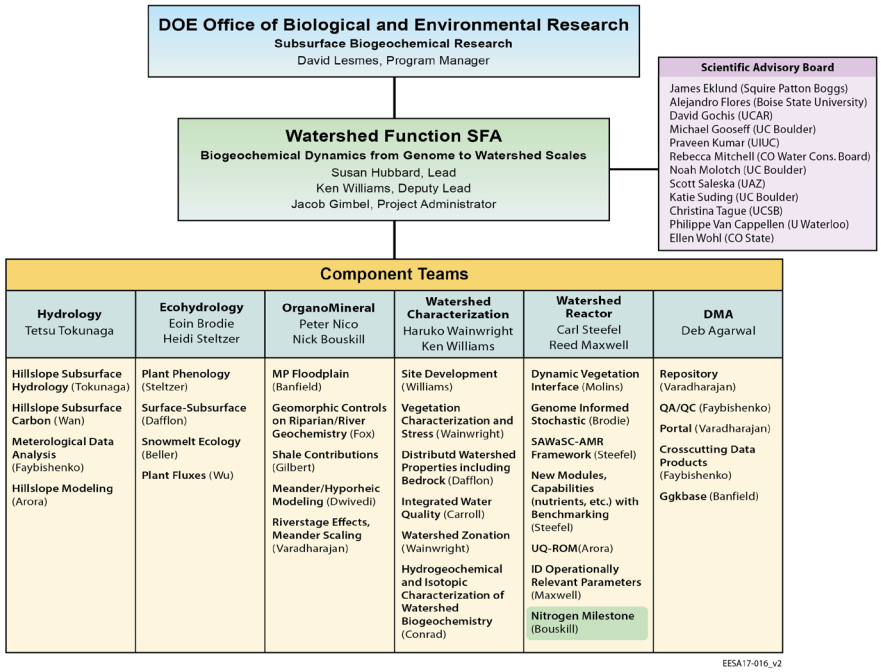


Figure 4. SFA organizational structure, showing structure, components and task leads as well as the Scientific Advisory Board.

listed below each component. A Scientific Advisory Board (SAB) has been assembled; SAB members and associated expertise are described on the SFA website at http://watershed.lbl.gov/people/scientific-advisory-board/.

The project integrates and benefits from leveraging offered by collaborating principle investigators from multiple institutions, who have independently funded projects affiliated with the SFA (Section 5). Over the years, BER funded science at SFA Colorado observatories (Rifle and East River, CO) have hosted 450 individuals to advance important discoveries and to develop and test new approaches, including researchers stemming from or including: 7 countries, 33 US states, 55 academic institutions, 73 postdocs, 66 graduate students, 16 federal, state and local government institutions (including USGS, NOAA, NASA, EPA) and 13 private sector organizations.

4.0 SFA PROGRESS

The Watershed Function SFA has realized significant progress during this reporting period. Achievements associated with select tasks, as well as overall progress toward reporting on investigations at Rifle CO conducted during the last phase and on meeting science question 3-year milestones. Effort this performance year has led to 41 publications (16 published in journals with an impact factor >5) and 50+ presentations. A summary of the Watershed Function SFA annual products is provided in Appendix VII, including journal publications, outreach, community service, invited presentations, and abstracts. During the 2017 AGU alone, the SFA led 8 sessions and gave 17 presentations. The Appendix also provides information about other relevant activity or recognition, such as workshops or special session organization, AGU Fellow and other awards, internal seed SFA projects, and relevant leadership positions and community service during this performance year.

While many FY18 tasks at East River are ongoing, several have already led to new insights and demonstrated outcomes**.** Figure A1 (in Appendix II) illustrates how different scientific components and FY18 tasks contribute to the supporting science questions. We have not encountered any challenges or discoveries in FY18 requiring a dramatic shift in focus or research priorities. We provide brief updates of select tasks associated with individual specific science questions, as indicated by the abbreviated task names listed in Figure A1.

4.1 Progress on Select Tasks Relevant to Question 1

: How do perturbations to individual watershed subsystems, including early snowmelt and drought, lead to changes in downgradient export of water, N, C and P from that subsystem? FY18 Tasks associated with this science question strive to gain an understanding of the hillslope and floodplain intensive sites. The investigations particularly focus on how these individual sites respond to seasonal perturbations, such as snowmelt or changes in river stage**.**

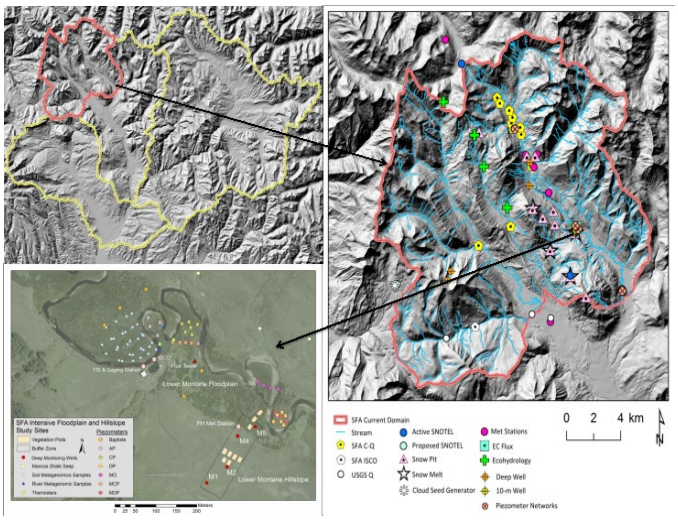


Figure 5. Intensive and satellite sites have been established that span a diversity of system compartments (e.g. hillslope, floodplain, bedrock) along gradients in elevation and climate/precipitation. These sites enable both long-term monitoring of natural processes & comparative manipulation experiments.

Site Development Activities (aligned with 'Intensive site development' task shown in Figure A1)

In an effort to link two critical subsystems within the study area – hillslopes and floodplains – a hydrologically interconnected intensive study site has been developed and expanded over the previous two years of SFA activities at East River (Fig. 5). The sites encompass an area of ~30 ha and include variations in lower montane vegetation composition and river morphology. The

interconnected study sites enable all Components of the SFA to pursue activities in tandem designed to decouple hydro-biogeochemical processes associated with both individual compartments (Q1), their connection (Q2) and their aggregation (Q3). Site development activities also focused on integrating the research actvities in the East River of a growing network of University and Federal Agency partners in a manner that greatly expands the intellectual and spatial footprint of the Watershed Function SFA. Activities included instrumentation and expansion of ecohydrology and biogeochemical monitoring plots, installation of floodplain piezometers and deep (90-100 m) bedrock monitoring wells, establishing dry and wet dust deposition monitoring stations, increased temporal sampling of metal-impacted streams, and upgrades and repairs to the meterological station network including the Eddy Covariance flux tower. In addition, five projects funded as part of DOE's Small Business Innovative Research (SBIR) are in various stages of implentation within the East River watershed.

Hillslope water flux measurements ('Subsurface hydro-biogeochemistry' task in Fig. A1)

Subsurface hydrologic responses to surface perturbations need to be understood to predict hillslope exports of water and nutrients into floodplains and rivers. This task focuses on the lower montane hillslope transect, instrumented using 10 m deep boreholes drilled through soil into Mancos Shale. Hydraulic potential measurements along the transect show that evapotranspiration influences the upper 2 m of soil and weathered shale. Measured time-dependent and depth-resolved hydraulic potentials along the hillslope (Fig. 6a), combined with measured hydraulic conductivities and estimates of hillslope recharge formed the basis for a simple model that constrained different subsurface components of baseflow (Fig. 6b). Baseflow through fractured shale zone (3 m down to about 40 m below the soil surface) continues at practically constant rate throughout the year. Snowmelt and water table rise generate large seasonal contributions to baseflow through the weathered shale zone (~1.2 to 3 m depth), and smaller fluxes over shorter periods through the soil. This analysis helps to constrain numerical modeling and is being combined with measured pore water solute concentration profiles to predict seasonal concentration-discharge trends for comparisons with measurements in the river.

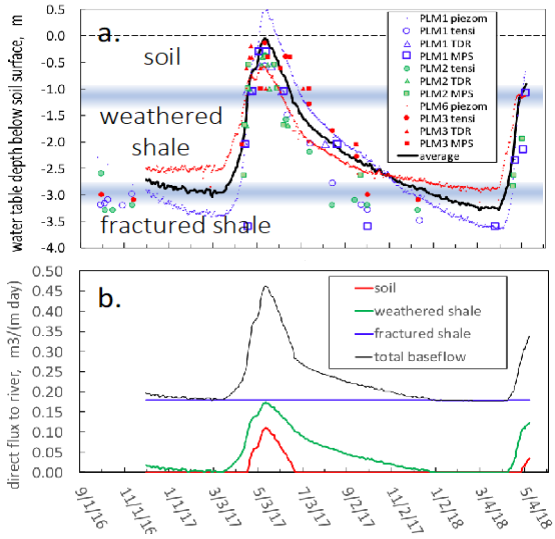


Figure 6. Hillslope subsurface water dynamics, showing (a.) seasonal variations in depths to the water table, and (b.) partitioning of baseflow through the deep fractured shale, sha

Surface-subsurface HBGC simulations along the hillslope intensive site ('Hillslope modeling')

This task focuses on using 2-D models to investigate the primary controls on water, carbon and nutrient fluxes along the intensive hillslope transect. An important goal here is to quantify hillslope and riparian contributions to streamflow under average hydrological conditions, as well as in response to higher/lower snowpack years. ToughReact results show that contributions from deeper subsurface regions are important to the overall hydrologic budget. Both measurements and model simulations show that increasingly negative matric potentials

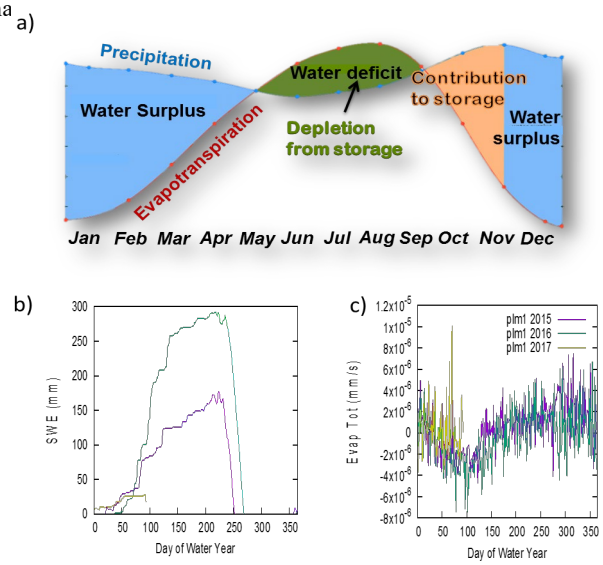


Figure 7. a) ToughReact simulations and observations provide a conceptual framework for ET demand throughout the year; ParFlow simulations show variations in **b)** snow water equivalent (SWE) and **c)** total ET across years.

develop in shallow subsurface regions during the growing season. This growing season demand (Fig. 7a) is significantly impacted by snowpack distribution and snowmelt timing. ParFlow-CLM results highlight the differences in evapotranspiration (ET) and snow water equivalent (SWE) across years with high and low snowpack (Fig. 7b, c). Future modeling efforts will focus on coupling the ToughReact 2D numerical model with ParFlow-CLM through top hydrologic boundary conditions so to accurately capture the linkages between evapotranspirative demand, surface runoff and biogeochemical fluxes.

Simulation of Vegetation and Soil Biogeochemical Dynamics at the Hillslope Intensive Site ('Hillslope BGC modeling')

This task focuses on examining the mechanisms underlying feedbacks between hydrologic and biogeochemical fluxes, microbial metabolism and vegetation phenology/physiology at the hillslope intensive site using a comprehensive mathematical process model, *ecosys*. We particularly focus on comparing these process couplings for an average hydrologic year (e.g., 2016) to variations due to a deep snow pack (as observed in 2017) or an unusually sparse and early melting snowpack (as observed in 2018). In low snow years, water potential data suggest that evapotranspiration driven pre-summer drought occurs post-snowmelt, water deficit in surface soils adversely impacts forb production and favors deep rooting shrubs altering vegetation N demand depending on slope. In high snow years, soil remains saturated. Topography and vegetation traits interact to influence plant species competition through access to water. Model results, consistent with observations, show that shrubs dominate on steeper slopes with forbs at shallow slopes. Model predictions further suggest that a longer growing season can be associated with a low snowpack year depending on the timing of post snowmelt precipitation. The model is able to capture snow water equivalent, snowmelt timing, shrub dominance, soil temperature and soil moisture trends across hillslope transect (Fig. 8). Ongoing modeling efforts will focus on reconciling microbial N versus plant N storage strategies.

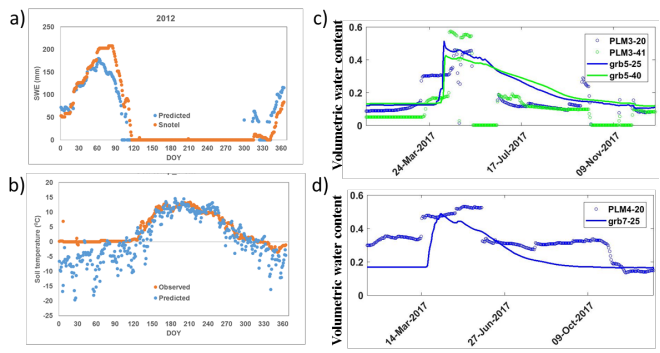


Figure 8. *ecosys* simulations compared to a) snow water equivalent (SWE), b) soil temperature and soil moisture trends at c) hillslope backslope and d) shoulder regions.

Snowmelt microbiology and biogeochemistry ('Snowmelt microbial ecology')

To enable a better understanding of the impacts of early snowmelt on export of N & C, this task has focused on collecting baseline data on hillslope biogeochemistry, particularly from snow accumulation through snowmelt, with a focus on measurements indicating microbially mediated processes (e.g., nitrification, N assimilation & release). Over the first 1.5 years of this project, ~450 samples at the Lower Montane site have been collected and analyzed for soil geochemistry (e.g., extractable and pore water NH_4^+, NO_3^-, amino acids, DOC and DON composition by FT-ICR MS) and microbiology (e.g., microbial biomass C and N and corresponding isotopic signatures; community structure based on 16S rRNA and ITS sequences; ongoing meta-genomic and metatranscriptomic analysis). In 2017, we observed a microbial biomass bloom during peak snowmelt (in May, later than expected) and a crash following loss of snow cover (in June)

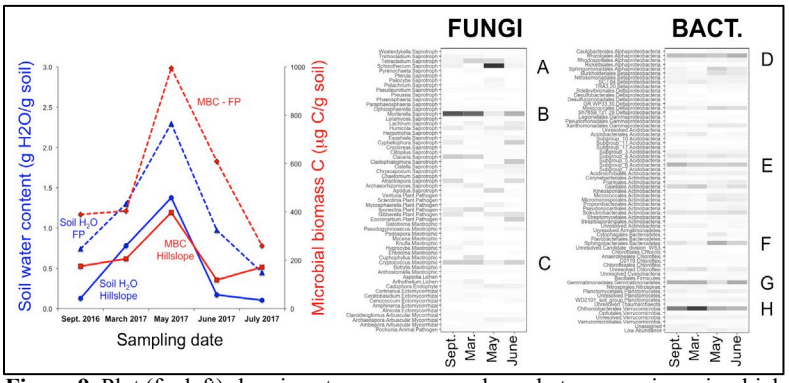


Figure 9. Plot (far left) showing strong correspondence between spring microbial biomass dynamics and snowmelt infiltration in hillslope and floodplain (FP) surface soils (0-5 cm), and heat maps (right) of microbial community dynamics in that soil horizon (shown for hillslope only). Particularly abundant & dynamic taxa are highlighted (A-H), including saprotrophic (A,B) and mixotrophic (C) fungi, as well as Acidobacteria (E) and Verrucomicrobia (H), whose importance in CO montane soils has been indicated previously.

along with dynamic changes in bacterial and fungal communities (Fig. 9). Microbial biomass N released between May and June accounted for a much greater portion of soil N flux than inorganic N species. Dramatic changes in pore water composition observed between May and June included a sharp increase in nitrate concentrations in June. Comparative analyses are underway for the snowmelt manipulation experiments conducted in April 2018.

Shale weathering and its controls on carbon, nutrients and metal fluxes ('Hillslope hydrology')
The Mancos shale is an important subsystem of the East River watershed because water-rock reactions can release nutrients and metals. We have made significant progress on understanding shale contributions to exports along three lines. The first is the characterization of depth-resolved elemental and mineralogical compositions (Fig. 10) of five sites along the hillslope intensive site. This effort included identification of three depth intervals characteristic of weathering and pedogenesis: the soil regolith typically spanning the 0-1.2 m depths, the weathering Mancos Shale zone at depths of 1.2-3.0 m, and the fractured parent Mancos Shale zone at depths greater than 3 m. We also quantified depth- and season-resolved C, nutrient, and metal concentrations in subsurface pore waters, and found that weathering in combination with hydraulic potentials control solute fluxes. These data will be used to constrain and validate the large-scale modeling of solute exports from the watershed. Finally, we quantified C inventories and fluxes to the groundwater, river, and atmosphere. Contrary to commonly accepted understanding, we found that the highest DOC concentrations at the hillslope site occur in the weathering zone, not in soil pore waters. We are using DOM compound classes and abundance (FTICR MS analyses at EMSL) and ^{14}C ages to investigate C behavior in the hillslope subsurface.

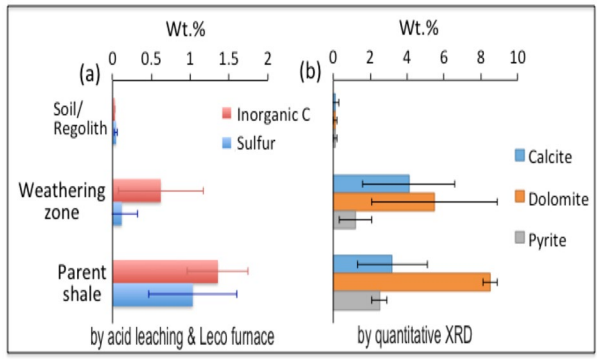


Figure 10. Examples of (a) elemental and (b) mineralogical compositions. Depths for the soil/regolith zone, weathered shale, and fractured shale are 0-1.2 m, 1.2-3.0 m, and below 3.0 m, respectively.

Redox Gradients Control Contaminant Release from Weathering Shale ('Shale weathering and controls on fluxes')
This task focuses on measuring weathering profiles in soil and rock and within individual fracture surfaces to infer the effects of water table variations on metal and nutrient release. Hillslope scale weathering profiles show a characteristic depletion of sulfides and carbonates from the surface to the groundwater table (Fig. 11a) as well as clay mineral transformations (data not shown). In addition, redox-active minerals (pyrite) and metals (Se, As, U) accumulate below the depth marking the transition between seasonally and permanently saturated zones. Fracture scale weathering profiles at 2 m depth revealed the loss of sulfur and non-redox-active metals (*e.g.* Zn^{2+}) from the weathered section but the retention of redox-active Se^0 and As at the pyrite weathering front (transition zone in Fig. 11b). At 2.5 m depth, Se and Mn additionally accumulate at the fracture surface (not shown). The data show that redox-sensitive metal inputs to the East River are limited in two ways. First, the shale pore-water during weathering has pH close to neutral and redox Eh very close to the Fe^{2+}/Fe^{3+} couple, limiting the release of Se and As. Second, oxidized Se and As transported from upper oxic regions into the anoxic groundwater are immobilized by reduction. We are currently developing a reactive transport model in CrunchFlow to describe the microscale weathering process as a prelude to publication.

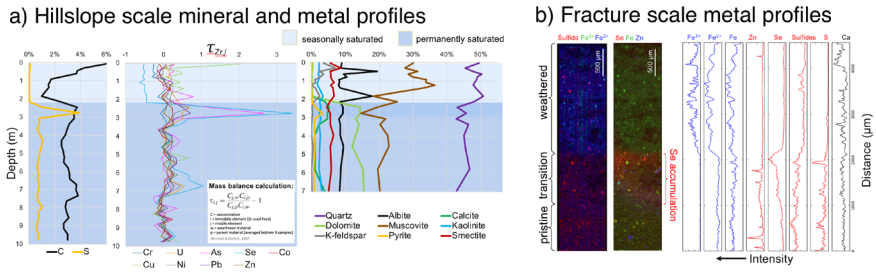


Figure 11. Patterns of Mancos shale weathering at East River drill location PLM6. **a)** Hillslope weathering profile of minerals and trace metals determined by bulk X-ray diffraction and composition analysis. **b)** Fracture weathering profile of redox sensitive metals on polished shale section at ~2 m depth determined by synchrotron microfocus X-ray fluorescence and X-ray absorption.

Floodplain Inter-Meander & Hyporheic Zone Modeling ('Meander modeling')

The overarching goal of this task is to quantify the contribution of the meanders to the downgradient export of water, C, N, and P in the floodplain and to develop a predictive understanding of how floodplain exports are impacted due to climatic perturbations, including early snowmelt and drought. We developed and incorporated a biotic and abiotic reaction network into the reactive transport simulator PFLOTRAN to examine the aggregated functioning of two active meanders of the floodplain intensive site. To quantify subsurface geochemical exports to the river and evaluate how transient hydrological conditions influence the lateral redox zonation within an intra-meander region, we performed several two-dimensional reactive flow and transport simulations. The simulation results demonstrate that highly dynamic redox gradients are predominantly driven by groundwater flux velocities resulting from river-stage fluctuations (Fig. 12). The simulation results also indicate that meanders act as a sink for carbon, both organic and inorganic, as well as for iron during high water conditions. In addition, subsurface exports are primarily hydrologically driven; however, biotic processes produce inorganic carbon and dissolved iron that are eventually released into the river during low water conditions.

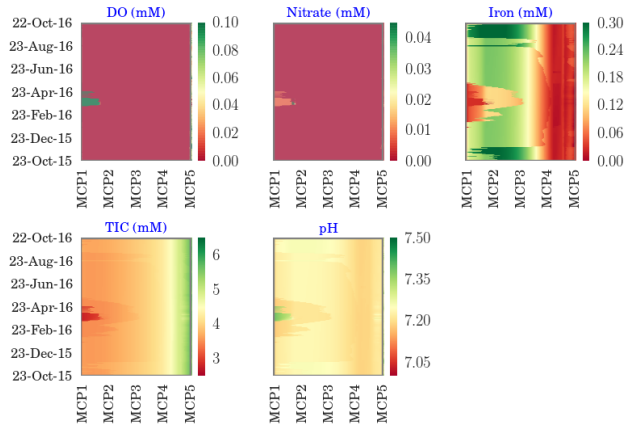


Figure 12. Simulated pH and geochemical species along a meander transect sand over time demonstrates redox zonation is dynamic and responds to river-stage fluctuations. MCPx indicates well locations along the transect (Dwivedi et al., 2017, Dwivedi et al., in review)

<u>4.2 Progress on Selected Tasks associated with Question 2</u>: How do early snowmelt and/or drought alter subsystem connectivity and fluid residence times within mountainous watersheds, including bedrock? The following FY18 tasks focused on exploring properties and processes in a region that encompasses the hillslope to floodplain subsystems.

Floodplain Meanders as a Motif for Upscaling Watershed Exports ('Upscaling meanders')

The specific objectives of this task are to (1) develop new approaches to quantify floodplain contributions over scales larger than a single meander and (2) examine hillslope-floodplain-meandering channel interactions and their threshold response, both in space and time. To quantify these exports over river reaches under transient conditions, we incorporated scaling behaviors into the East River reactive transport modeling framework. We hypothesized that residence times and meander geometry can be used to upscale geochemical fluxes from meander to river reach scales. The preliminary simulation results (Fig. 13) show that hillslope-floodplain-meandering channel interactions produce micro-zones of high biogeochemical activity and lateral and vertical redox zonation within the intrameander regions. Results of the high-resolution, 3-D models capture this complex biogeochemical response at the meander scale with non-unidirectional flow paths, fluxes and suggest that sinuosity and hyporheic flow paths significantly impact carbon and nitrogen export into the stream system. The simulation results further demonstrated that intermediate frequencies (~3 months) of water table fluctuations exert a significant control on the export of groundwater nutrients, nitrogen, and carbon, both organic and inorganic, to the stream on the downstream side and over reach scales.

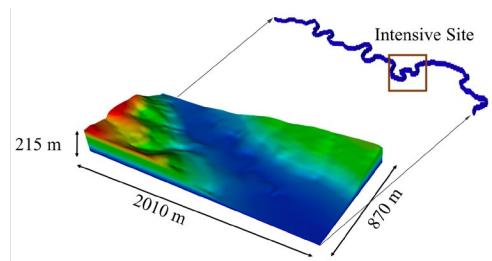


Figure 13. Scaling behaviors were incorporated into a floodplain reactive transport model permitting extension of the impact of meander-associated hydro-biogeochemistry over river reach scales.

Quantification and Comparison of Microbial Community Structure at Different Intensive Sites ('Meander Microbio')

This task focuses on the analysis of samples obtained from the intersection of a meander-associated location at the floodplain intensive site (ERML, Fig. 14) and the base of the hillslope intensive site (PLM4, Fig. 14), which is about 350 m downstream from ERML. In order to understand potential connectivity between the two intensive sites, we are using genome-resolved metagenomics and metatranscriptomics of soil microbial communities. Specifically, we are investigating the composition and activity of dominant microbial communities involved in biogeochemical cycles. Near-complete genomes (684) were obtained from both sites. Out of these, 150 genomes (75 non-redundant) were of Betaproteobacteria, Deltaproteobacteria and Nitrospirae species, which were found to be the most abundant taxa. Metabolic predictions indicate that some of the Betaproteobacteria (abundant in top soil) can oxidize thiosulfate to sulfate, and some Nitrospirae (found in proximity to the water table) can use sulfur as the electron donor. Community composition was compared among sites using a ribosomal protein S3 (rpS3) marker gene. Preliminary analyses show that the most abundant species in the microbial communities are ubiquitous (Fig. 14). In topsoil from the two sites (ERML and PLM4), Betaproteobacteria and Deltaproteobacteria are the first and second most abundant Proteobacteria classes, respectively. Nitrospirae were relatively more abundant at 65 cm in PLM4, whereas Deltaproteobacteria were most abundant at 90 cm (below the water table). Overall the results suggest that the microbial community structure of meander-associated riparian zone topsoil resembles that of the floodplain at the toe of the hillslope site but differs from deeper samples. Ongoing analysis of other hillslope sites (PLM0-PLM3), as well a comparative analysis of the two adjoining intensive study sites (hillslope and meander associated sites), is underway and expected to generate insights regarding the microbial connectivity within and between the two subsystems.

Figure 14. Relative abundance was estimated for ERML (n= 31), and PLM4 (n=9) taken in 2016. Sequences of rpS3 genes were clustered (99% similarity) and reads from all samples were mapped to the scaffolds to calculate breadth and abundance.

Root Zone Thermo-Hydrological Responses to Precipitation and Snow Experimentation ('Plant-soil sensing')

To monitor thermo-hydrological dynamics and their impacts on nutrient, water, and carbon fluxes, we installed and analyzed samples from a monitoring network that traversed the hillslope to floodplain intensive sites (Fig. 15). More than 30 boreholes were installed with soil lysimeters and sensors to a depth of 1.5 meters, covering the entire root zone, surface soil and the underlying saprolite. Data spanning the 2016-2017 and 2017-2018 water years revealed significant variability of the soil thermo-hydrological responses to changes in annual precipitation. Specifically, prolonged (> 5 months) surface soil layer frozen down to > 50 cm was observed from 2017-2018 year, contrasting significantly with the warm and wet soil under the snow for the 2016-2017 year. Such a contrast was also observed in the soil hydrological dynamics, where a much shorter snowmelt-induced wet pulse (<1 month) was observed in the soil compared to last year (> 2 months). Indicated by the sensor data, snow manipulation successfully advanced the snow-free date on the experimental plots by 10 days when compared to the control plots, which was further augmented by a naturally occurring two-week advance compared to last year. Besides the significant contrast of soil thermo-hydrology between the last two years, CO_2 monitoring data has indicated the impact of the frozen soil condition on surface flux and its link with changing hydrology during snowmelt. These results provide critical data for understanding the plant-biome response to natural and manipulated hydrological perturbations.

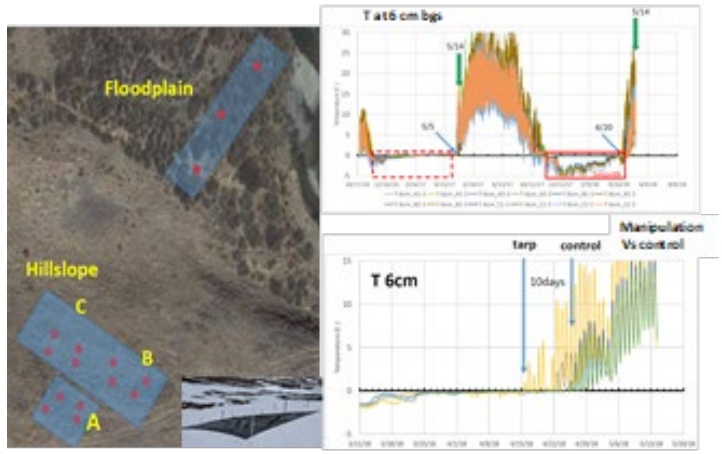


Figure 15. Hillslope-to-floodplain transects thermo- hydrological dynamics during the last two years, including impacts from snowmelt manipulation.

Machine Learning with UAV Data to quantify Covariance of Vegetation, Soil Moisture and Topography ('Veg characterization')

In this task, we characterized the heterogeneity of plant communities and quantified the covariance with key environmental variables, such as topography and soil moisture, spanning the floodplain and hillslope intensive sites. We developed a high-resolution fusion framework that implements a spectral and structural data classification strategy using UAV-based data that was based on support vector machine and morphological contextual analysis. We then compared the covariance between interpreted vegetation types, soil moisture, and topographic metrics along the hillslope transect. The analysis clearly revealed a strong correlation between the spatial distribution of the plant communities, soil electrical conductivity, and topographic characteristics (Fig 16). Veratrum and riparian shrubland consistently populate depressions or flat areas with slope close to level and high soil moisture, while plants such as sagebrush grow along ridges or moderate steep areas with limited soil moisture. These observations demonstrate the potential of the proposed framework for effective integration of remote sensing and geophysical data for revealing interactions between above and below ground critical zone compartments.

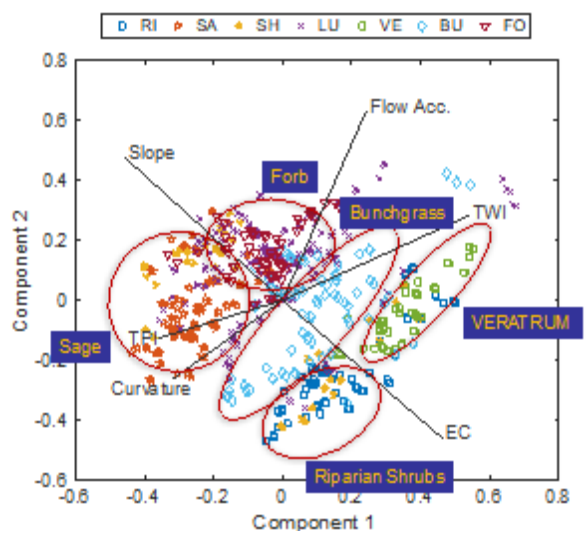


Figure 16. Biplot from principal component analysis, showing the clusters of topographic metrics and electrical conductivity (EC) according to plant functional types (Falco et al., in review).

Relationship between Snow Depth, Vegetation Dynamics and Slope Aspect explored using Time-Lapse UAV ('UAV and machine learning')

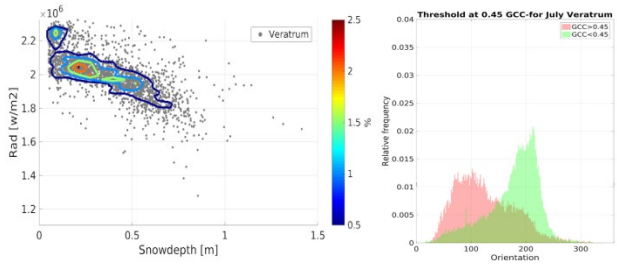


Figure 17. (left) Snow depth (here at veratrum location) in early April is strongly influenced by the cumulative radiation. (right) Highest radiation (on south facing slopes) is linked to earliest senescence of veratrum (shown by low GCC in July).

Quantifying the distribution of snow depth, vegetation type and dynamics, soil characteristics, and land surface properties at relevant spatiotemporal scales is critical to investigate watershed responses to perturbations. In this task, we analyzed time-lapse UAV data collected from the NE facing hillslope through the floodplain intensive sites and the adjacent SW facing hillslope. Seven UAV optical survey campaigns were performed over eight months, including periods of snowmelt, growing season and plant senescence. The inferred time-lapse digital surface model (DSM) and multi-spectral (Red, Green, Blue, Red edge and Near infrared) orthomosaics provided spatiotemporal maps of vegetation height, snow thickness and of normalized vegetation indexes such as Green Chromatic Coordinate (GCC). The time-slices were used to investigate relationships between landscape position, snow dynamics and vegetation dynamics. Results show that the snow dynamics (snow-depth and snow-melt) are highly correlated with cumulative radiation (an integrator of slope, orientation and sun position) from January to May, with only minimal and local influence of non-tree plant type on snow distribution (Fig. 17). We also observed different seasonal dynamics between various plant types as well as in each plant type. Indeed, the cumulative radiation and the flow accumulation are interpreted to be key components controlling plant growth-senescence timing. For example, Veratrum has the fastest growth and the earliest senescence compared to other plant types and shows a faster cycle where radiation is the highest. These observations will be combined with hydrogeophysical and biogeophysical information obtained along the hillslope intensive transects.

Monitoring of Above-and-Below-Ground Co-dynamics using Remote/Autonomous Sensors ('Above and below co-dynamics')

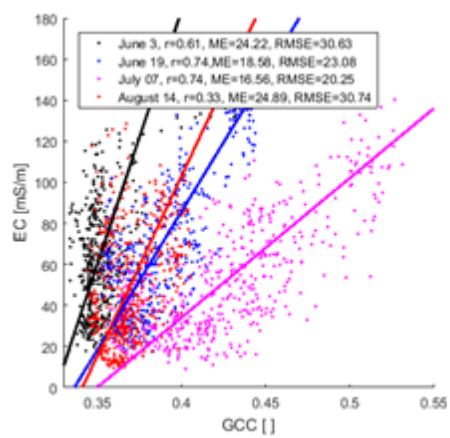


Figure 18. Temporally variable relationship between soil electrical conductivity and green chromatic coordinate along a hillslope to floodplain transect.

Improving the predictive understanding of how perturbations to individual watershed subsystems, including early snowmelt and drought lead to changes in ecosystem dynamics and feedbacks between soil and vegetation processes requires quantification of the spatiotemporal co-variability between soil, surface and vegetation properties. This task focused on the development and analysis of time-lapse UAV-based multi-spectral imagery (such as described above) and a distributed autonomous network of soil moisture sensors and daily-acquired electrical resistivity tomography (ERT), installed along a transect connecting the hillslope to floodplain intensive sites, to evaluate the linkages between plant spectral signature, topography and soil properties. Results indicate that i) the soil electrical conductivity (EC) of the top 40 cm is highly correlated over time and is sensing both the change in water content over time and the soil characteristics, including soil compaction and clay content; ii) the relationship between the green chromatic coordinate (GCC, normalized vegetation index for plant vigor and density) and the soil EC varies over time and that the strongest correlation coefficient (0.74) occurs at the peak of the growing season between mid-June and mid-July (Fig. 18); iii) the greenness-soil electrical conductivity relationship is stronger than any relationships between vegetation index, topographic metrics and soil characteristics. Multi-dimensional relationships will be further evaluated to partition the control of various soil properties on plant type and vigor. These results are also promising for predicting soil properties from aerial measurements once selecting the right timing.

Sulfur isotopic indicators of redox conditions in groundwater ('Sulfur isotopic indicators of groundwater redox poise')

Groundwater redox conditions govern transport and the chemical state of critical elements (C, N, metals) from the watershed. Isotopic monitoring of redox-sensitive compounds (e.g., NO_3, SO_4, CH_4, U) in groundwater and surface water in the East River watershed are being used to track movement of water through different subsurface environments. The sulfur isotope composition of sulfate has proven to be a sensitive indicator of the fraction of water that has passed through highly reducing zones in the subsurface. Cretaceous Mancos Shale that contains pyrite with an average $\delta^{34}S$ of -20‰ underlies a large part of the watershed. Oxidation of this pyrite by oxygenated surface water produces sulfate with a similar sulfur isotope ratio and releases metals such as U. This effect has been observed in the sulfur isotope ratios of sulfate along a hillslope-to-floodplain transect hosted by Mancos Shale (Figure 19). The net result is that the $\delta^{34}S$ values of sulfate in the East River and its tributaries are lower during spring snowmelt but increase during the summer and fall as drainage into the river system becomes increasingly dominated by contributions from deeper, anaerobic groundwater. This conclusion is supported by ^{222}Rn concentrations indicating zones of groundwater incursion into the river. These results suggest that pyrite in shale-dominated systems has a significant role in limiting oxygen transport into the subsurface, maintaining reducing conditions in deeper groundwater, limiting mobility of redox-sensitive metals as evidenced by observed U isotopic shifts related to reduction of U^{+6} to U^{+4}.

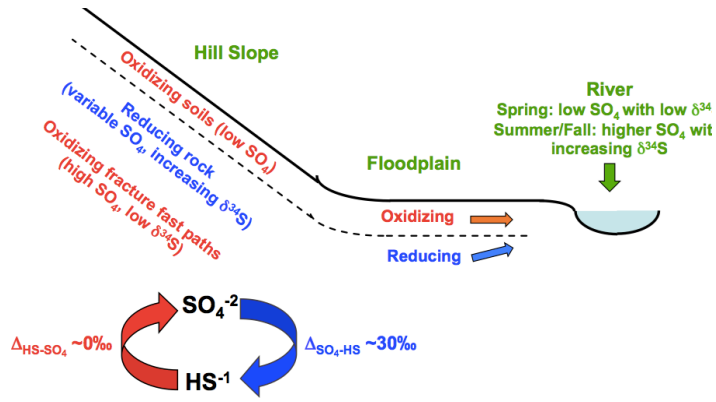


Figure 19. Microbial sulfate reduction produces sulfide with much lower sulfur isotope ratios leading to enrichment of ^{34}S in the residual sulfate, whereas sulfide oxidation produces little to no shift between the sulfur isotopic composition of the produced sulfate and the residual sulfide.

<u>4.3. Progress on Select Tasks associated with Question 3</u>: How do interactions between vegetation, hydrology, subsurface biogeochemistry and geology, particularly in response to perturbations, vary along diverse watershed gradients and contribute to aggregated C, N, P and metal exports from the watershed? Tasks associated with this science question use both data analysis and modelling approaches to gain an understanding of distributed watershed properties and processes across larger watershed regions (beyond intensive sites), and how those aggregate to yield an integrated watershed concentration-discharge signature.

Plant Phenology across an Elevation Gradient ('Plant phenology across gradient')

Through observing plant phenology and microclimate, we are investigating how plants in mountain systems time their growth in relation to key climate drivers, such as snowmelt and drought. We are monitoring the timing of plant leaf emergence immediately following loss of snow cover at five stations along an elevation gradient in the watershed ranging from 9,100-11,800 feet (Fig. 20). Through multiple weekly visits during the snow-free season, we have also tracked the timing of leaf expansion, flowering, and leaf and plant senescence. Observations are made for all species (each circle in Fig. 20 represents a species) within each of two 1m x 1m subplots located within the six study plots at each of the five sites. Early snowmelt at the lower three elevations leads to the initiation of plant growth in mid-May through early June. We find that across these sites, plot greening is offset due to the timing of snowmelt but overlaps across the three elevations. Leaf expansion occurs concurrently in early June across all three sites. In contrast, plot greening in the upper two elevations occurred in early- to mid-July, decoupling growth at these elevations from the lower ones. We considered this a threshold phenological response across the watershed, likely due to a combination of factors that lead to substantially greater snow fall and accumulation, and thus later snowmelt and plant growth above ~11,000 feet elevation. While these findings were expected, the timing and duration of the decoupled plant growth across elevation was not.

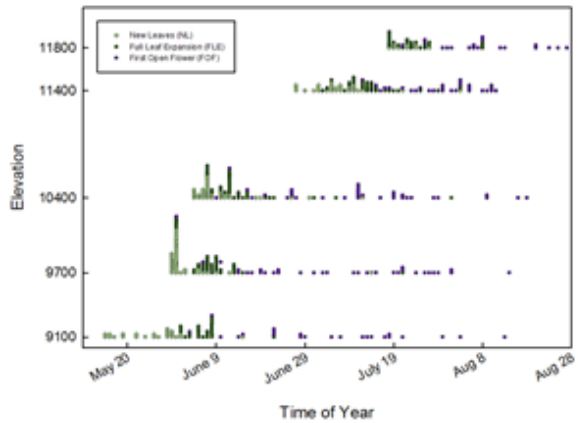


Figure 20. The timing of plant growth varies across elevation due to 2018 snow melt date and plant evolutionary strategies.

Early Snowmelt Manipulation across an Elevation Gradient ('Snowmelt manipulation experiments')
In temperate mountain watersheds, snowmelt is a major hydrologic event associated with large annual fluxes of nitrogen among soils-plants-microbes, as well as a major driver of nitrogen export from watersheds. Through an early snowmelt experiment, we aim to decouple soil-plant-microbe relationships to assess consequences in terms of the timing and magnitude of nutrient release. Black fabric is placed on the snow surface in three 10m x 14m experimental plots at four of our study sites across the same elevation gradient described above, with examples shown in Fig. 21. The fabric is removed when plots are 80% snow free, with remaining snow in the experimental plots melting rapidly. Our aim was to have experimental plots be snow free concurrent with control plots at the next lower elevation. A key driver of coupled soil-plant-microbe interactions would be similar for contrasting elevations and their associated plant and microbial communities.

Figure 21. A view of the lower subalpine study site during the snowmelt manipulation in April 2018 and its consequence for earlier green-up in mid-May, when the hillslope had become snow free.

Winter 2017 was typical of winters past in the Colorado Rocky Mountains with above average snowfall and persistent snow into June and July. Winter 2018 contrasted substantially with reduced snowfall, especially early in the season. The snowmelt experiment began in 2018 to allow one year of pre-treatment data across all plots. At each site, the treatment created an 8–12-day advance in the timing of snowmelt. We were also able to achieve the intended aim for similar snow free dates across paired elevations between earlier snowmelt and control plots. Clear differences within a site can be seen in greenness of early snowmelt vs. control plots. Graminoid and forb leaf expansion occurred earlier due to earlier snow free conditions, and several species have emergent leaves at snowmelt even when snow is lost early. Soil and microbial analysis is underway to determine if aboveground shifts in plant growth correspond with belowground shifts or whether growth is decoupled and nutrient release and availability are shifted. Such data are supplemented with soil microclimate and phenocam data to link soil physical and chemical properties with seasonal greening.

End-Member Mixing Analysis to Identify Seasonal Stream Sources ('End-member analysis')

To isolate first-order controls on seasonal streamflow generation within highly heterogeneous, snow-dominated basins of the Colorado River, we employed a multivariate statistical approach of end-member mixing analysis (EMMA) using a suite of daily chemical and isotopic observations. Mixing models are developed across 11 nested basins (0.4 km^2 to 85 km^2) spanning a gradient of climatological, physical and geological characteristics. Hydrograph separation using rain, snow and groundwater as end-members indicates that seasonal contributions of groundwater to streams is significant. Mean annual groundwater flux ranges from 12% to 33% while maximum groundwater contributions of 17% to 50% occur during baseflow. We found groundwater recharge increases in basins of high relief and within the upper sub-alpine where maximum snow accumulation is coincident with reduced conifer cover and lower canopy densities (Fig. 22). The mixing model developed for the furthest downstream site did not transfer to upstream basins. The resulting error in predicted stream concentrations points toward weathering reactions as a function of source rock and seasonal shifts in flow path. Additionally, the potential for microbial sulfate reduction in floodplain sediments along a low gradient, meandering portion of the river is sufficient to modify hillslope sulfate contributions and alter mixing ratios in the analysis. Soil flushing in response to snowmelt is not included as an end-member but is identified as an important mechanism for release of solutes.

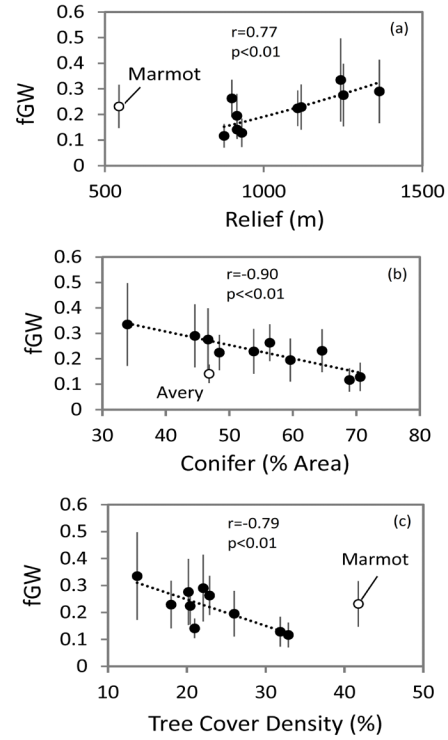


Figure 22. Fraction of groundwater in stream water fGW (annual mean ± range) with respect to (a) relief, (b) conifer by area, and (c) tree cover density. Basins excluded shown as a white symbol (Carroll et al., 2018)

Quantification of Spatiotemporal Variability of Evapotranspiration at the East River Watershed ('ET spatiotemporal watershed variability')

ET is a key component of the water balance, influencing water resource management, carbon and nitrogen cycles, and ecosystem diversity. However, accurate predictions of ET are challenging due to dependence on complex interactions of highly variable water-heat-energy fluxes. We developed a novel approach to combine semi-empirical methods and numerical simulations of spatiotemporal variations of evapotranspiration (ET) over the scale of the East River Watershed. Spatiotemporal variations of ET at the East River watershed were predicted using semi-empirical formulae and numerical simulations using the Community Land Model (CLM) for the period of 1993-2014 (Fig. 23). The model was validated by comparing its outputs with ET estimated based on (a) a modified Budyko's model, and (b) a watershed-scale water balance. Simulation results show that 55% of annual precipitation at the East River watershed is lost to ET, with 75% of ET during the summer months (May to September). Transpiration is estimated to be ~50% of total ET, largely exceeding soil evaporation (32%) and canopy evaporation (18%). ET spatial variability is governed by closely correlated effects of elevation, air temperature, and vegetation. An important conclusion is ET is greater at middle elevations (2950-3200

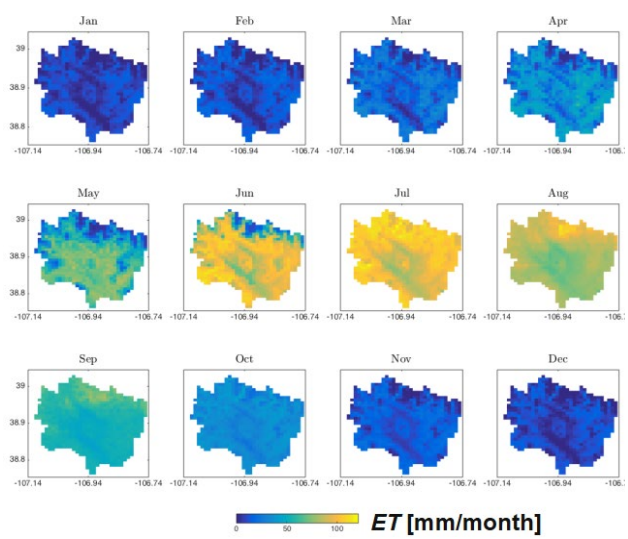


Figure 23. Spatiotemporal estimation of ET over the watershed and over time (Tran et al., 2018 in review).

m), and smaller along the river valley (<2750 m) and at high elevations (>3900 m). We found that soil properties also influenced ET, being slightly higher in areas with finer texture soil. ET is largest over the south, southwest and southeast-facing topographic aspects. Results of this study are being used as inputs for hydrological and biogeochemical modeling of the East River watershed and will be used for evaluating spatial statistics of ET across the East River watershed.

Historical Watershed Sensitivity to Perturbations such as Drought and Early Snowmelt ('Watershed sensitivity to drought and early snowmelt')

Historical data provide rich information to identify and quantify the sensitivity of snow, streamflow and vegetation to climate perturbations such as early snowmelt and drought. We used a data-driven approach to better understand the coupling between inter-annual variability in temperature, snow and plant community dynamics, and stream discharge. This approach is based heavily on a set of datasets typically available throughout the US, providing a powerful approach to link remote sensing techniques with long-term monitoring of temperature, snowfall, plant, and streamflow dynamics. We applied the method to historical spatiotemporal datasets available at the site, including the SNOTEL data, Landsat-based normalized difference vegetation index (NDVI) and streamflow data. Although snow distribution and NDVI are spatially heterogeneous, the inter-annual variability and temporal responses are spatially consistent, providing an opportunity to quantify the effect of temperature at the catchment-scale (Fig. 24). We demonstrate our approach within the East River watershed where the changes in plant communities and their dynamics have been extensively documented over the past fourteen years. Results indicated that temperature – particularly spring temperature – has a significant control not only on the timing of snowmelt, plant NDVI, and peak flow but also on the magnitude of peak NDVI, peak flow and annual discharge. Monthly temperature in spring explains the variability of snowmelt by the equivalent standard deviation of 3.4-4.4 days, and total discharge by 10–11%. In addition, the high correlation among June temperature, peak NDVI and annual discharge suggests a primary role of spring evapotranspiration on plant community phenology, productivity, and streamflow volume. On the other hand, summer monsoon precipitation does not contribute significantly to annual discharge, further emphasizing the importance of snowmelt dates.

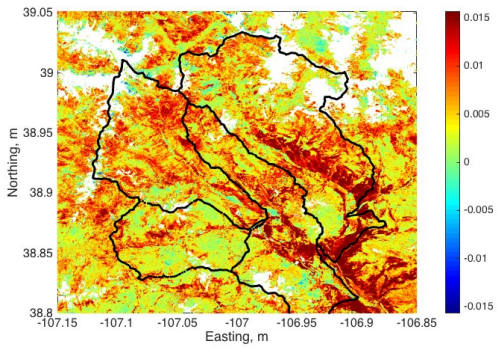


Figure 24. Sensitivity of Landsat Peak NDVI to June Palmer Drought index in the four watersheds (Wainwright et al., in review)

Decadal trends in solute and nutrient export across watershed scales of the United States ('Decadal trends in solute/nutrient export across watershed')

Over the last few decades, many studies have reported increases in global flows of nitrogen due to increased fertilizer application and deposition. Despite many efforts to attribute stream nitrogen fluxes to nitrogen inputs and inter-annual climatic variability (i.e. precipitation driven stream exports), in many watersheds, nitrogen fluxes have systematically declined. In this task, we test a new hypothesis regarding watershed-scale nutrient and solute flux trends that examines stream fluxes as an indicator of a watershed's eco-hydrological response to systematic long-term change. We use a data-driven approach scaled by hydrologic unit code boundaries to correlate exogenous climate drivers and watershed physical and eco-hydrological characteristics to streamflow concentration, fluxes, and nutrient dynamics. We examined trends in streamflow N, DOC, DO, P, stream temperature, and vegetation NDVI across the East River and across HUC2-HUC8 scales within the United States. Results (Fig. 25) show that at the East River and across many US watersheds, nitrogen concentrations and fluxes have decreased over the past 30 years despite large variability in N deposition, precipitation, and discharge, particularly in high-elevation headwater watersheds above 8,000ft. We found that watershed NDVI and streamflow temperature, which are indicators of biogeochemical and ecohydrological activity, were strongly linked to nitrogen fluxes suggesting a long-term systematic change in watershed scale ecosystem functioning. Stream fluxes from upstream to downstream show scaling behavior with watershed characteristics such as drainage area, and peak flow. This scaling relationship was found to be dependent on the antecedent dry or wet conditions of

the watershed as a whole as measured by precipitation. Our data-driven approach provides a powerful scale-based view linking these important eco-hydrological metrics to watersheds biogeochemical processing

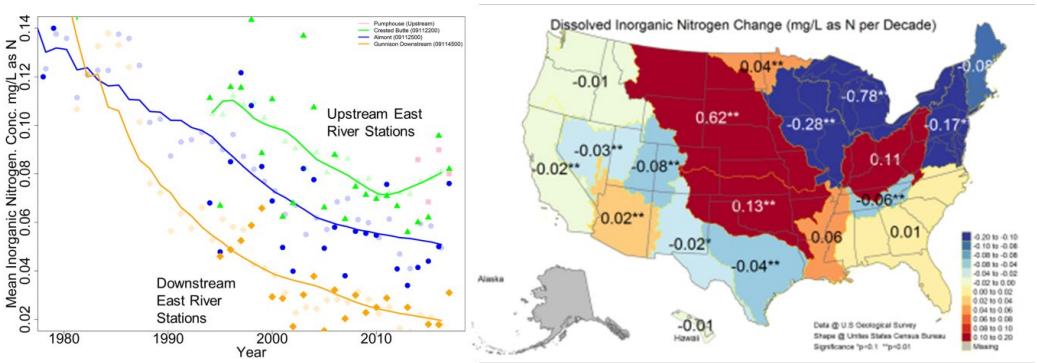


Figure 25. Trends in Dissolved Inorganic Nitrogen Concentrations for the East River (left) and for the entire US (right). (Newcomer et al., in preparation).

across the United States.

Toward Watershed Scale Mechanistic Reactive Transport Simulations: Development of Modeling Capabilities ('Model development')

We used ATS-AMANZI to simulate integrated hydrological processes, winter snowpack, and subsequent snowmelt that controls stream chemistry at the Copper Creek (CC) and Lower Triangle region (LTR) sub-catchments of the East River watersheds (Fig. 26). CC is a high elevation sub-catchment that contributes flow to the East River approximately 25% annually. The ultimate goal is not only the simulation of integrated hydrology at the watershed scale but also simulation of reactive transport processes. For this purpose, a code that is capable of solving transport and biogeochemical reactions is needed, and many activities are underway to achieve this. For example, a reaction network previously developed as part of this SFA for biotic and abiotic processes in the Rifle floodplain (Arora et al, 2015; Dwivedi et al, 2018) was used in a relatively simple domain geometry under dynamic flow conditions at the East River. With support from the IDEAS project, the ATS integrated hydrology code has been expanded to include transport both in the subsurface and surface components. The Alquimia interface, an interoperable interface designed to provide biogeochemical processes to flow/transport models, was used to represent geochemical processes including chemical weathering of rock and solute transport as well as mineral precipitation and dissolution in the models in the CC and LTR regions. In addition, interoperable development has made it possible to enable the biogeochemical capabilities of PFlotran and CrunchFlow via the use of the Alquimia interface.

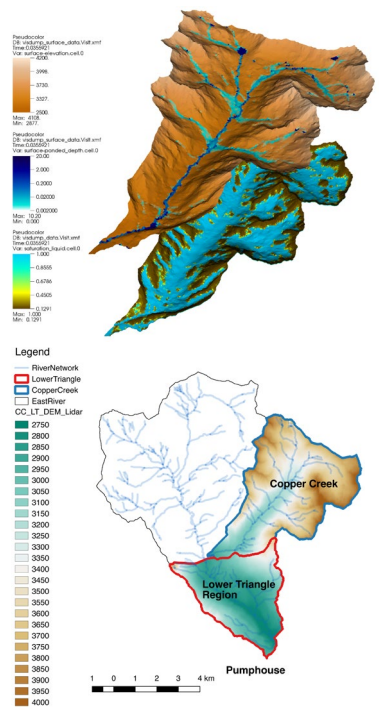
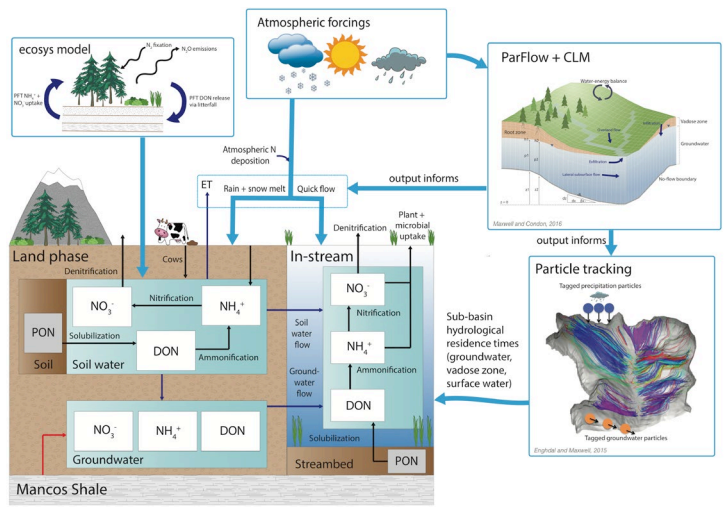


Figure 26. Top: simulated ponded water and saturation. Bottom: CC and LTR regions of the watershed are being used to test new reactive transport codes and tools, as well as to explore aggregated behavior.

We also used a 100 m resolution ParFlow-CLM model to simulate changes in the hydrologic budget of the lower triangle sub-watershed that were quantified for historical water years (WYs) representative of different end-member climate conditions. Results reveal that not only are the magnitudes of infiltration and evapotranspiration dependent on the climate of the water year but that precipitation and spring temperature affect the timing of groundwater replenishment and plant activity. As a novel pairing of physically based and lumped parameter modeling, a Lagrangian particle tracking technique is currently being coupled to this ParFlow-CLM model output to determine solute residences times required as input into a Markov chain Monte Carlo nitrogen model.

East River Watershed-scale Semi-Distributed Mechanistic Nitrogen Chain of Models ('N Milestone')
This task focuses on developing a watershed-scale 'chain' of models to quantify the aggregated behavior of nitrogen resolved at sub-basin scale. This task incorporates data from field and laboratory measurements and coupling to existing land and hydrological modeling efforts within the SFA. This semi-distributed model will be used to address questions related to the SFA 3-year nitrogen milestone such as: what factors control the input, transformation and loss of nitrogen at the watershed scale, and what explains the multi-decadal observed decrease in N export? Is watershed net primary productivity supported by weathering of the Mancos Shale? How do climate-driven processes (e.g., shrubification) impact N cycling and fluxes from the watershed?

Figure 27. Conceptual model framework of East River chain of models**.**



Our model chain consists of a watershed-scale semi-distributed mechanistic N model that quantifies major sources, sinks, and transformations of NO_3^-, NH_4^+, and dissolved organic N (DON) in the stream, soil and groundwater (Fig. 27). Despite the breadth of questions this model will be able to address, we have made a deliberate point of insuring the model is not over-parameterized by keeping the number of calibration parameters <25, compared with 50-100s in most watershed nutrient models. Sub-basin residence times characterizing surface and subsurface hydrologic dynamics were parameterized using the three-dimensional integrated hydrologic model ParFlow-CLM and a Lagrangian particle tracking approach. The *ecosys* model was used to constrain plant and microbial N uptake and release rates. The model chain was calibrated against riverine N time series of nitrate concentrations using a Markov Chain Monte Carlo algorithm, according to the Goodman and Weare (2010) algorithm. The overall approach of coupling multiple models and auto-calibrating using Bayesian techniques represents the most state-of-the-art watershed-scale nutrient model currently in existence. The use of a Bayesian modeling framework will additionally allow for a detailed quantification of model uncertainty, which is conspicuously lacking in the vast majority of watershed nutrient models.

Remote Sensing for Characterizing Hydrologic, Geologic, and Vegetation Parameters at the Watershed Scale ('Watershed remote sensing and other sitewide acquisitions')

Two basin-scale remote sensing datasets were collected this performance period that focused on imaging surface and subsurface physical properties, with a third underway related to vegetation characterization. NASA's Airborne Snow Observatory (ASO) was used to quantify spatial and temporal variations in snow depth and snow water equivalent (SWE) (Fig. 28) over the Ohio Creek, East River, and Taylor River basins. Given the importance of this information for improved water forecasting, funds external to the SFA for data collection and processing were obtained through stakeholder engagement with the State of Colorado Water Conservation Board and the Upper Gunnison Water Conservancy District. Airborne electromagnetic and radiometric data collected over the Coal Creek-Slate River-Washington Gulch-East River study domain was undertaken by USGS collaborators, with the data used to quantify variations in subsurface lithology and structural geology, as well as bedrock properties relevant to metal content and fracture density. Flight planning and design of a tandem ground-sampling campaign are underway tied to a June 2018 hyperspectral imaging overflight undertaken using the Airborne Observation Platform (AOP) operated by the National Ecological Observation Network (NEON). This data will be used to upscale ground-based measurements of vegetation composition and tissue chemistry to the full watershed study domain.

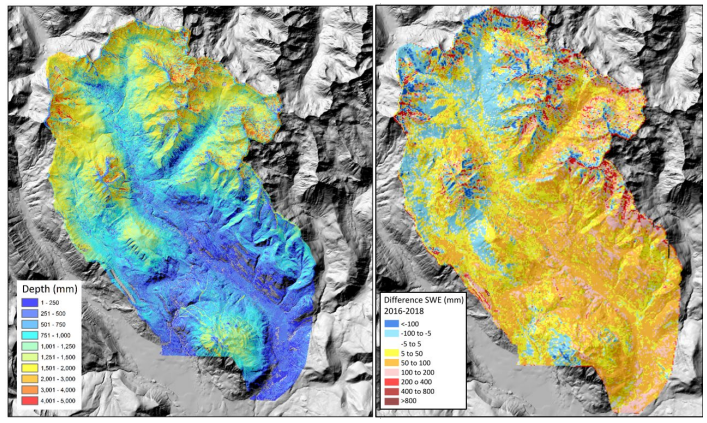


Figure 28. Snow depths determined by NASA's ASO on March 30, 2018 (left); difference in ASO-derived SWE between the 4-4-16 and 3-30-18 flights (right).

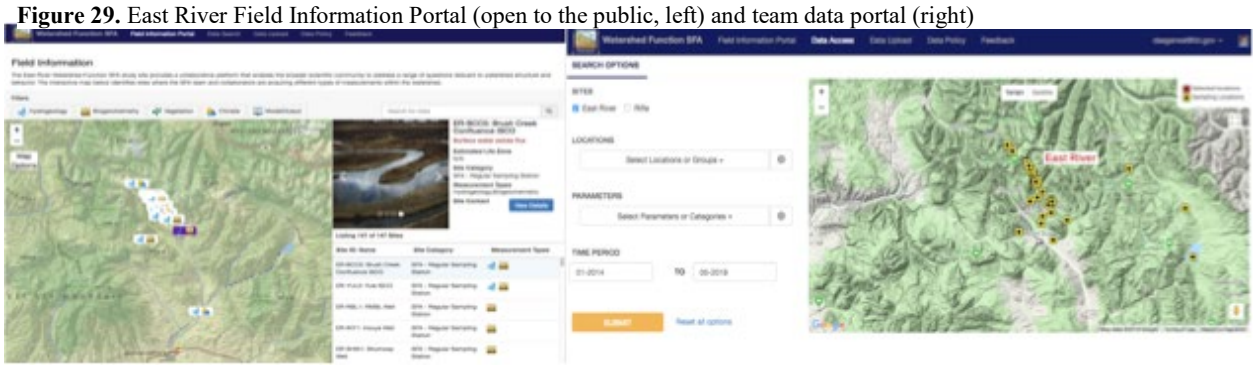
Data Management and Assimilation ('Data Packaging system', 'Data QC', 'Data access', 'Basin-3D', 'Community portal')

The objectives of the DMA component of the SFA are to enable science by: (1) managing and archiving the data collected by the project, and releasing those data publicly with appropriate citation information, (2) enabling the project team and the broader community to find where, when and what types of data are being collected through an interactive portal, (3) performing quality assurance and quality control of priority datasets, and (4) creating an data integration engine and search portal that can help retrieve, fuse and visualize the diverse data for further synthesis and analysis.

This year, data management capabilities were focused on the improvement of data accessibility and quality, including: maintenance and troubleshooting of existing sensor data including weather stations and wells; QA/QC processing of the data; implementation and release of a data packaging system; development of a meteorological database; and development of an initial controlled vocabulary. One example is the extensive data QA/QC flagging, cleaning, and corrections of time series data that have been carried out for the 17 meteorological stations. To extend the duration of time series of meteorological data, QA/QC of the past 20-30 years, using the datasets retrieved from NARR/Reanalysis, WCC DRI, and PRISM databases. Vetted data were applied for the hillslope modeling and sensitivity analysis of evapotranspiration and infiltration, using numerical codes CLM, *ecosys* and ParFlow, and the PLM groundwater levels via implementation of a back-end architecture that supports sensor specific time dependent conversion parameters. Examples include correction of an fDOM sensor and the time dependent correction of elevation for the PLM6 water level sensor by programmatically applying a shift to the level 0 data using a location and sensor parameter specific correction. This year we supported 6 weather stations, 10 instrumented wells, and about 30 multilevel soil instruments. A campaign to collect and update measurement locations was undertaken and the interactive portals were updated to incorporate this information.

The project data integration and search infrastructure, BASIN-3D, was updated to enable integration of model data output and released as version 1.1. The Community portal that provides information about measurements being made at the various study sites was updated to connect to BASIN-3D. Data preservation and distribution are being enabled by a web portal that allows authorized users (team members and collaborators) to upload and download data files as packages. The tool requires users to enter metadata needed to enable web searches and obtain custom SFA DOIs for citation. The data package tool enables early data sharing amongst the team and compliance with the DOE Data Management requirements. Users can search and download data even before they are ingested into the database. Contributors are notified of downloads and can update data as needed. See https://wfsfa-data.lbl.gov/watershed

Figure 29. East River Field Information Portal (open to the public, left) and team data portal (right)



The SFA database currently holds the metadata of monitoring posts and observational time series, as well as geochemical data comprising about 14 GB of data including 2731 geochemical water samples from 28 locations with more than 70,000 analyte/location pairs and over hundred million time points, value pairs of physical sensors. Datasets have been submitted as data packages (currently about 6.2 GB) and tens of GB of separately stored remote sensed data (LIDAR and multispectral imagery). All of the datasets are accessible through either our API or web interfaces (https://eastriver.pafbeta.subsurfaceinsights.com/).

5. STAFFING/BUDGET SUMMARY AND LAB INVESTMENTS IN THE WATERSHED

Budget allocations were distributed in FY18 as a function of components and component research is organized into tasks that align with the supporting science questions (SSQs). Berkeley Lab Watershed SFA staff and their associated time allocation are provided in the Appendix. The significant remote sensing and drilling costs during this performance year were burdened under the 'equipment/management' budget category.

Berkeley Lab has made a number of substantial investments aligned with the Watershed SFA this year. As described in the Appendix, lab investments include four LDRD projects associated with the Watershed SFA and associated labwide Microbes-to-Biomes and Water-Energy initiatives. Importantly, Berkeley Laboratory is making a substantial investment in the planning and Site preparation for the BioEPIC ("Biological and Environmental Program Integration Center") building, which was approved for CD-0 in March of 2018. The Laboratory has also invested in an EcoSENSE "SMART" Soils testbed and associated instrumentation, which will provide a foundation for a virtual ecosystem testbed that will be tied to the Watershed SFA (and ideally to other BER observatories in outyears). The Watershed project has also made a number of investments in S&T and associated experimental and simulation capabilities during this performance period. Investments in airborne datasets and other resources were described in Section 4, and additional investments are described in the Appendix. Importantly, the SFA offered a Collaborative Mini-Grant Opportunity (CMO) in FY18, which solicited ideas from within and beyond the SFA team for enhancing impact of SFA research through seeding projects that connect the SFA with other BER-relevant activities and initiatives. The three chosen projects will enhance linkage of the Watershed SFA with: the FATES effort of the NGEE-Tropics project (CMO SFA PI Lara Kueppers), with KBase (CMO SFA PI Romy Chakraborty) and with BioEPIC EcoSENSE (CMO SFA PI Yuxin Wu).

Research activities performed by the Watershed Function SFA are greatly enhanced through complementary investigations led by a network of externally funded partners. These investigations are tightly coordinated with SFA component and task leads to avoid duplication of effort and to extend and/or expand studies of broad relevance to the SFA. During this performance period, the Watershed SFA collaborated with 19 entities at the East River Site, including PIs from 3 private sector organizations, 5 National, Federal or other research Laboratories, and many universities. A brief synopsis of these FY18 activities is provided in the Appendix. Also provided in the Appendix are descriptions of substantial community activities, Berkeley Lab investments, and activities that the Watershed SFA has undertaken to enhance early career and collaborator involvement in watershed science at the East River.

APPENDICES

Appendix I. References for Literature Cited in Section 4

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21. Wainwright, H. M., S. Trutner, K. H. Williams, S. S. Hubbard, H. Steltzer, and B. J. Enquist (submitted), Mapping Fore-summer Drought Sensitivity of Ecosystem Functioning in Mountainous Watersheds: Spatial Heterogeneity and Geological-Geomorphological Control, *Environ Res Lett*.
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Appendix II. FY18 Key tasks

Figure A1 illustrates how different scientific components contribute to the supporting science questions. Cells with colored shading indicate FY18 activity, which primarily focused during this reporting period on Questions 1 and 3.

Six Supporting Science Questions	Component Based FY18 Tasks					
	Hydrology	EcoHydrology	OrganoMineral Dynamics	Watershed Characterization	Watershed Reactor	Data Management & Assimilation
Response of watershed subsytems to perturbations (hillslope and floodplain)	• Hillslope Hydrology • Subsurface Hydro-biogeochemistry • Hillslope modeling	• Snowmelt microbial ecology • Hillslope BGC modeling	• Meander modeling • Shale weathering and controls on fluxes	• Intensive Site Development		
Connectivity between subsytems	• Meander microbio	• Above and below ground sensing of co-dynamics • Plant-soil sensing	• Sulfur isotopic indicators of groundwater redox poise	• Veg characterization • UAV and machine learning	• Upscale meanders	
Aggregated watershed response	• ET spatiotemporal watershed variability	• Plant phenology across gradient • Snowmelt manipulation experiments		• Watershed sensitivity to drought and early snowmelt • End-member analysis • Watershed remote sensing and other sitewide acquistions	• Decadal trends in solute/nutrient export across watershed • N milestone • Lower east river integrated modeling • Model chain for simulating watershed nitrogen cycle	• Data packaging system • Data QC • Data access • Basin-3D • Community portal
Sufficient but minimum fine-scale information						
Impacted catchment responses						
Operational forecasting						

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Figure A1. Matrix indicating specific FY18 component-based tasks and their association with supporting science questions. Colored cells indicate FY18 activity, the majority of which are associated with the first and third question. Several tasks active in FY18 are not listed; progress on tasks that are listed is provided in section 4.

Appendix II. Collaborative research activities with external investigators

Research activities performed by the Watershed Function SFA are greatly enhanced through complementary investigations led by a network of externally funded University, USGS, and National Laboratory partners. These investigations are tightly coordinated with SFA component and task leads to avoid duplication of effort and to extend and/or expand studies of broad relevance to the SFA. Brief synopses of these activities over the reporting period follow.

1. **Jared Balik** (North Carolina State Univ.); **Corey Lawrence** (USGS): Linking spatial variations in hillslope and floodplain soil phosphorus pools with temporal variations in soluble reactive phosphorus concentrations within the East River mainstem and Rock Creek. [Funding source: NSF-GRIP]
2. **John Bargar** (SLAC): Sampling of organic matter-rich transient reduced zone sediments along the Slate River and Coal Creek drainages in support of SLAC's "Groundwater Quality" SFA project. [Funding source: DOE-BER]
3. **Max Berkelhammer** (Univ. Illinois, Chicago); **Chris Still** (Oregon State Univ.): Evaluating and quantifying through predictive models the biotic and abiotic controls on space and time dynamics of transpiration in the East River watershed. [Funding source: DOE-BER]
4. **David Bomse** (Mesa Photonic LLC): Development and field testing of portable systems for (a) the isotopic analysis of soil gases and (b) low power soil gas analysis. [Funding sources: DOE-SBIR]
5. **Martin Briggs** (USGS): Identification of groundwater upwelling zones within the East River and Coal Creek drainages to assess their role in mediating metal oxide transformations and metals mobility. Analysis of variations in stream and surface water temperatures in the East River and Oh-Be-Joyful Creek drainages using thermal imagery obtained through handheld and UAV infrared

cameras to isolate lateral inputs of groundwater along the river corridors. [Funding source: DOE-BER]

6. **Rosemary Carroll** (DRI): Groundwater age dating using multiple tracers to constrain watershed transit time distributions, with samples for dating collected from both deep groundwater wells and springs/seeps. [Funding source: USGS]
7. **Dana Chadwick** (Stanford Univ.): Ground-based sampling and analysis of vegetation, litter, and soils associated with imaging data collected by NEON's Airborne Observation Platform. [Funding source: NSF postdoctoral fellowship; NSF-EAGER]
8. **Rick Colwell** (Oregon State Univ.); **Laura Lapham** (Univ. Maryland): Development and deployment of autonomous, continuous flow osmo-samplers to collect samples for geochemical analysis in deep boreholes and under-ice riverine locations. [Funding source: DOE-BER]
9. **Jeff Deems** (CU Boulder): Utilization of multi-scale, seasonal snowpack observations and modelling to more accurately account for water and solute storage and fluxes within the upper Gunnison basin.
10. **Scott Fendorf** (Stanford); Marco Keiluweit (UMASS): Research examining redox controls on organic matter stability within floodplain sediments along the East River transect from the Pumphouse intensive study site to the Brush Creek confluence satellite site. [Funding source: DOE-BER]
11. **Alejandro Flores** (Boise State Univ.); **Rosemary Carroll** (Desert Research Institute): Working with Berkeley Lab partners to advance the ability to accurately predict the spatiotemporal distribution of snow cover and water content across multiple scales by combining land-atmosphere models with operational multi-satellite remote sensing data. [Funding source: DOE-BER]
12. **Ruby Ghosh** (OptiO2 Inc.): Development and field testing of optical methods for quantifying temporal variations in dissolved oxygen concentrations in solid phase substrates including stream bed sediments and hillslope soils. [Funding source: DOE-SBIR]
13. **Elliot Grunewald** (Vista Clara, Inc.): Field testing and validation of dynamic nuclear magnetic resonance (NMR) logging technologies for the high-resolution measurement of hydrogeologic properties in fractured bedrock. [Funding source: DOE-SBIR]
14. **Marco Keiluweit** (UMASS): Investigating root influences on the mobilization, mineralization and export of mineral-bound soil organic matter within floodplain and hillslope soils of the East River watershed. [Funding source: DOE-BER].
15. **Li Li** (PSU): Reactive transport model development describing seasonal excursions in aqueous metals and carbon export within the Coal Creek drainage using detailed concentration-discharge analysis of key metals and biologically critical elements. [Funding source: DOE-BER]
16. **Lee Liberty** (Boise State Univ.): Quantifying regolith, rock and fluid distributions within the greater East River watershed via a multicomponent seismic imaging approach. [Funding source: DOE-BER]
17. **Kate Maher** (Stanford): Micro-catchment studies within the upper East River drainage focused on hillslope controls on carbon and nitrogen transport through a combination of data collection and reactive transport modelling, with results tied to the synoptic SFA modelling effort. [Funding source: DOE-BER]
18. **Reed Maxwell** (CSM); **Dave Gochis** (NCAR): Installation of observational facilities within the watershed (Eddy Covariance flux tower; meteorological station) to create a high-elevation carbon-flux observational testbed for simulating carbon and water fluxes using a coupled land surface hydrology-high resolution atmospheric modelling system (WRF-Hydro-ParFlow). [Funding sources: DOE-BER; RMBL]
19. **Burke Minsley, Lyndsay Ball** (USGS): Use of airborne electromagnetic, magnetic, and radiometric datasets to development a structural and compositional subsurface model of the East River watershed. [Funding source: USGS]
20. **Don Nuzzio** (Analytical Instrument Systems Inc.): Development and field validation of portable impedance spectroscopy equipment to provide both synoptic ('prospecting') and fixed location monitoring for aqueous concentrations of oxygen, sulfide, lead, zinc, and cadmium. [Funding source: DOE-SBIR]

21. **Peggy O'Day** (UC Merced): Quantification of atmospheric inputs of phosphorus to the watershed and assessment of its bioavailability along an elevation gradient within the watershed. Research activities are performed with complementary studies at the Southern Sierra Critical Zone Observatory. [Funding source: DOE-BER]
22. **Anamika Ray** (Innosense LLC): Development and field validation of a portable nanowire platform for quasi real-time and ultrasensitive detection of microbes. [Funding source: DOE-SBIR]
23. **Daniella Rempe** (Univ. Texas, Austin): Quantifying the importance of the bedrock vadose zone as an ecologically significant hydrologic reservoir that strongly influences watershed response to perturbations. [Funding source: DOE-BER]
24. **Joel Rowland** (LANL): Geomorphological studies along the low gradient, meandering reach of the East River drainage examining the role of floodplains in regulating the export and retention of solid phase carbon tied to erosion, deposition, and accretion. Extensive use of airborne imagery data is enabling detailed characterization of decadal variations in floodplain and riparian zone evolution. [Funding source: DOE-BER Early Career]
25. **Audrey Sawyer (**Ohio State Univ.**)** Quantifying controls of dynamic water table fluctuations on reactive solute transport near the groundwater-surface water interface. [Funding source: NSF Early Career]
26. **Josh Sharp** (CSM): Assessment of the impact of early snowmelt on beetle-impacted spruce needle litter degradation pathways and subsequent nutrient release to soils and atmosphere. Both non-manipulated (lower montane) and manipulated (lower subalpine) studies are being used to assess snowmelt drivers impacting relevant biogeochemical pathways. [Funding source: DOE-BER]
27. **Alexis Sitchler** (Colorado School of Mines): Examining the impact of contact metamorphism on Mancos shale physical properties and its role in impacting East River morphological evolution. [Funding source: RMBL]
28. **McKenzie Skiles** (Univ. Utah); **Janice Brahney** (Utah State Univ.); **David Gochis** (NCAR): Constraining the physical understanding of aerosol loading, biogeochemistry, and snowmelt hydrology from hillslope to watershed scale within the East River watershed and its surrounding drainages. [Funding source: DOE-BER]
29. **Roelof Versteeg** (Subsurface Insights): Development of (a) cloud-based data management tool for watershed and terrestrial ecosystem data and (b) real time measurement systems for monitoring and imaging coupled surface/subsurface processes.
30. **Rich Wanty, Andy Manning** (USGS): Identification of deep groundwater controls on metals release within the Slate River drainage through collection of hydrogeochemical data and bedrock hydrologic properties obtained through deep drilling in the Redwell Basin. [Funding source: DOE-BER]
31. **Mike Wilkins** (Ohio State Univ.): Quantifying the importance of vertical hyporheic exchange in driving biogeochemical reactions within streambed sediments in the East River drainage. Data collection includes vertical variations in streambed temperature, redox conditions and microbial community composition. [Funding source: DOE-BER]

Appendix III. SFA Products List

Aggregated Publication Metrics. Watershed Function SFA publications have been cited more than 3800 times since 2012. The field-weighted citation impact (FWCI) of publications in this period is 3.83, meaning on average, SFA publications have been cited 3.83 times more than comparable publications in the publications' respective fields (FWCI also accounts for age of publication, whereas citation count does not).

Published during this Performance Year. Research during this performance year has led to 41 publications (16 published in journals with an impact factor >5) and 50+ presentations. The table below shows the published and in press publications for this performance year.

Journal	JIF 5yr	Count of articles

Nature	41.577	2
Nature Geoscience	14.391	1
Nature Microbiology	14.174	1
Nature Communications	12.353	1
ISME Journal	9.52	1
Earth-Science Reviews	7.491	1
Environmental Science & Technology	6.653	8
Msystems	5.75	1
Geochimica Et Cosmochimica Acta	4.69	1
Science of the Total Environment	4.61	2
Water Resources Research	4.361	2
Scientific Reports	4.122	2
Frontiers in Microbiology	4.019	2
Microbial Ecology	3.614	1
Advances in Water Resources	3.512	1
Hydrological Processes	3.181	2
Journal of Environmental Sciences	3.12	1
Organic Geochemistry	2.81	1
Environmental Science: Processes & Impacts	2.6	1
Geophysical Journal International	2.528	1
Geophysics	2.368	1
Vadose Zone Journal	2.23	1
Groundwater	1.9	1
Handbook of Metal-Microbe Interactions and Bioremediation: Principle and applications for toxic metals	n/a	1
The heaviest metals: Science and technology in Actinides and beyond	n/a	1
Genome Announcements	n/a	1
Procedia Earth and Planetary Science	n/a	2
Grand Total		**41**

Select 2018 Submitted (not counted in table above)

1. Berkelhammer, M., C. Still, F. Ritter, M. Winnick, K. H. Williams, L. Anderson, R. Carroll, and S. Nash (submitted), Hydrologic memory drives persistence in forest water use strategies, *Proceedings of the National Academy of Sciences of the United States of America*.
2. Dwivedi, D., et al. (in review), Geochemical Exports to River from the Intra-Meander Hyporheic Zone under Transient Hydrologic Conditions: East River Mountainous Watershed, Colorado, *Water Resour Res*.
3. Falco, N., H. Wainwright, B. Dafflon, E. Léger, J. Peterson, H. Steltzer, C. Wilmer, J. C. Rowland, K. H. Williams, and S. S. Hubbard (under revision), High-resolution characterization of a mountainous floodplain-hillslope vegetation community and associated covariance with soil moisture and topography using remote sensing and machine learning approaches, *Journal of Geophysical Research - Biogeosciences*.

4. Feng, Z., R. W. H. Carroll, R. Schumer, C. Harman, D. Wilusz, and K. H. Williams (submitted), Hydrologic connectivity in snow-dominated basins as a function of climate, *Water Resour Res*.
5. Foster, L., and R. M. Maxwell (submitted), Using sensitivity analysis and model resolution to scale effective hydraulic conductivity and Manning's n parameters in a mountain headwater catchment, *Hydrol Process*.
6. Hubbard, S. S., et al. (in revision), The East River, CO Watershed: A Mountainous Community Testbed for Improving Predictive Understanding of Multi-Scale Hydrological-Biogeochemical Dynamics, *Vadose Zone Journal*.
7. Tran, A. P., J. Rungee, B. Faybishenko, B. Dafflon, and S. S. Hubbard (in revision), Quantifying Evapotranspiration and Analyzing Its Spatiotemporal Variability in a Mountainous Watershed, *Hydrology and Earth System Sciences*.
8. Wainwright, H. M., S. Trutner, K. H. Williams, S. S. Hubbard, H. Steltzer, and B. J. Enquist (submitted), Mapping Fore-summer Drought Sensitivity of Ecosystem Functioning in Mountainous Watersheds: Spatial Heterogeneity and Geological-Geomorphological Control, *Environmental Research Letters*.
9. Wainwright, H. M., S. Trutner, E. Woodburn, M. Newcommer, K. H. Williams, S. S. Hubbard, and R. Carroll (submitted), A Statistical Approach to Deconvolve the Seasonal Relationships between Precipitation and Temperature on Snow and Streamflow Metrics within a Snow-dominated Headwater Catchment, *Hydrol Process*.
10. Wan, J., et al. (submitted), Observed deep vadose zone carbon fluxes from a semi-arid floodplain contradict current Earth System Model predictions, *Environ Sci Technol*.
11. Zhi, W., L. Li, W. Dong, W. Brown, J. P. Kaye, C. I. Steefel, and K. H. Williams (submitted), Disproportionately high solute export during snowmelt in a mining-impacted watershed, *Environ Sci Technol*.

2018 Publications, including in press manuscripts

1. Anantharaman, K., et al. (2018), Expanded diversity of microbial groups that shape the dissimilatory sulfur cycle, *The ISME Journal*, DOI: 10.1038/s41396-018-0078-0.
2. Arora, B., J. A. Davis, N. F. Spycher, W. Dong, and H. M. Wainwright (2018), Comparison of Electrostatic and Non-Electrostatic Models for U(VI) Sorption on Aquifer Sediments, *Groundwater*, *56*(1), 73-86, DOI: 10.1111/gwat.12551.
3. Carroll, R. W. H., L. A. Bearup, W. Brown, W. Dong, M. Bill, and K. H. Willlams (2018), Factors Controlling Seasonal Groundwater and Solute Flux from Snow-Dominated Basins, *Hydrol Process*, DOI: 10.1002/hyp.13151.
4. Christensen, J. N., et al. (2018), Using strontium isotopes to evaluate the spatial variation of groundwater recharge, *Sci Total Environ*, *637-638*, 672-685, DOI: 10.1016/j.scitotenv.2018.05.019.
5. Danesh-Yazdi, M., J. Klaus, L. E. Condon, and R. M. Maxwell (2018), Bridging the gap between numerical solutions of travel time distributions and analytical storage selection functions, *Hydrol Process*, *32*(8), 1063-1076, DOI: 10.1002/hyp.11481.
6. Dwivedi, D., B. Arora, C. I. Steefel, B. Dafflon, and R. Versteeg (2018), Hot Spots and Hot Moments of Nitrogen in a Riparian Corridor, *Water Resour Res*, *54*(1), 205-222, DOI: 10.1002/2017wr022346.
7. Hao, Z., H. A. Bechtel, T. Kneafsey, B. Gilbert, and P. S. Nico (2018), Cross-Scale Molecular Analysis of Chemical Heterogeneity in Shale Rocks, *Scientific Reports*, *8*, DOI: 10.1038/s41598-018-20365-6.
8. Holmes, D. E., R. Orelana, L. Giloteaux, L.-Y. Wang, P. Shrestha, K. Williams, D. R. Lovley, and A.-E. Rotaru (2018), Potential for Methanosarcina to Contribute to Uranium Reduction during Acetate-Promoted Groundwater Bioremediation, *Microbial Ecology*, DOI: 10.1007/s00248-018-1165-5.
9. Jemison, N. E., A. E. Shiel, T. M. Johnson, C. C. Lundstrom, P. E. Long, and K. H. Williams (2018), Field Application of U-238/U-235 Measurements to Detect Reoxidation and Mobilization of U(IV), *Environ Sci Technol*, *52*(6), 3422-3430, DOI: 10.1021/acs.est.7b05162.
10. Orozco, A. F., J. Gallistl, M. Bücker, and K. H. Williams (2018), Decay curve analysis for data error quantification in time-domain induced polarization imaging, *GEOPHYSICS*, *83*(2), E75-E86, DOI: 10.1190/geo2016-0714.1.

11. Schmidt, F., H. M. Wainwright, B. Faybishenko, M. Denham, and C. Eddy-Dilek, In-Situ Monitoring of Groundwater Contamination for Sustainable Remediation Using the Kalman Filter, in press, *Environmental Science and Technologies*.
12. Tokunaga, T.K., Y. Kim, J. Wan, M. Bill, M. Conrad and W. Dong, Method for controlling temperature profiles and water table depths in laboratory sediment columns. In press, Vadose Zone Journal.
13. Wainwright, H. M., B. Arora, B. Faybishenko, S. Molins, S. S. Hubbard, K. Lipnikov, D. Moulton, G. Flach, C. Eddy-Dilek, and M. Denham (2018), Sustainable Remediation in Complex Geologic Systems, in *The heaviest metals: Science and technology in Actinides and beyond*, edited by W. Evans and T. P. Hanusa.

2017 Publications

14. Arora, B., D. Dwivedi, N. Spycher, and C. Steefel (2017), On Modeling CO2 Dynamics in a Flood Plain Aquifer, *Procedia Earth and Planetary Science*, *17*, 408-411, DOI: 10.1016/j.proeps.2016.12.103.
15. Arora, B., Y. Cheng, E. King, N. Bouskill, and E. Brodie (2017), Chapter 27: Modeling microbial energetics and community dynamics, in *Handbook of Metal-Microbe Interactions and Bioremediation: Principle and applications for toxic metals*, edited, CRC Taylor and Francis Group.
16. Banfield, J. F., K. Anantharaman, K. H. Williams, and B. C. Thomas (2017), Complete 4.55-Megabase-Pair Genome of "Candidatus Fluviicola riflensis," Curated from Short-Read Metagenomic Sequences, *Genome Announcements*, *5*(47), DOI: 10.1128/genomeA.01299-17.
17. Bone, S. E., M. R. Cahill, M. E. Jones, S. Fendorf, J. Davis, K. H. Williams, and J. R. Bargar (2017), Oxidative Uranium Release from Anoxic Sediments under Diffusion-Limited Conditions, *Environ Sci Technol*, *51*(19), 11039-11047, DOI: 10.1021/acs.est.7b02241.
18. Boye, K., V. Noel, M. M. Tfaily, S. E. Bone, K. H. Williams, J. R. Bargar, and S. Fendorf (2017), Thermodynamically controlled preservation of organic carbon in floodplains, *Nature Geoscience*, *10*(6), 415-419, DOI: 10.1038/ngeo2940.
19. Burstein, D., L. B. Harrington, S. C. Strutt, A. J. Probst, K. Anantharaman, B. C. Thomas, J. A. Doudna, and J. F. Banfield (2017), New CRISPR–Cas systems from uncultivated microbes, *Nature*, *542*(7640), 237-241, DOI: 10.1038/nature21059.
20. Castelle, C. J., C. T. Brown, B. C. Thomas, K. H. Williams, and J. F. Banfield (2017), Unusual respiratory capacity and nitrogen metabolism in a Parcubacterium (OD1) of the Candidate Phyla Radiation, *Scientific Reports*, *7*, 40101, DOI: 10.1038/srep40101.
21. Daugherty, E. E., B. Gilbert, P. S. Nico, and T. Borch (2017), Complexation and Redox Buffering of Iron(II) by Dissolved Organic Matter, *Environ Sci Technol*, *51*(19), 11096-11104, DOI: 10.1021/acs.est.7b03152.
22. Delahaye, B., D. Eveillard, and N. Bouskill (2017), On the Power of Uncertainties in Microbial System Modeling: No Need to Hide Them Anymore, *Msystems*, *2*(6), DOI: 10.1128/mSystems.00169-17.
23. Dong, W., J. Wan, T. K. Tokunaga, B. Gilbert, and K. H. Williams (2017), Transport and humification of dissolved organic matter within a semi-arid floodplain, *Journal of Environmental Sciences*, *57*, 24-32, DOI: 10.1016/j.jes.2016.12.011.
24. Dwivedi, D., I. C. Steefel, B. Arora, and G. Bisht (2017), Impact of Intra-meander Hyporheic Flow on Nitrogen Cycling, *Procedia Earth and Planetary Science*, *17*, 404-407, DOI: 10.1016/j.proeps.2016.12.102.
25. Faybishenko, B. (2017), Detecting dynamic causal inference in nonlinear two-phase fracture flow, *Advances in Water Resources*, *106*, 111-120, DOI: 10.1016/j.advwatres.2017.02.011.
26. Fox, P. M., P. S. Nico, M. M. Tfaily, K. Heckman, and J. A. Davis (2017), Characterization of natural organic matter in low-carbon sediments: Extraction and analytical approaches, *Organic Geochemistry*, *114*, 12-22, DOI: 10.1016/j.orggeochem.2017.08.009.
27. Jewell, T. N. M., U. Karaoz, M. Bill, R. Chakraborty, E. L. Brodie, K. H. Williams, and H. R. Beller (2017), Metatranscriptomic Analysis Reveals Unexpectedly Diverse Microbial Metabolism in a Biogeochemical Hot Spot in an Alluvial Aquifer, *Frontiers in Microbiology*, *8*(40), DOI: 10.3389/fmicb.2017.00040.

28. Keiluweit, M., T. Wanzek, M. Kleber, P. Nico, and S. Fendorf (2017), Anaerobic microsites have an unaccounted role in soil carbon stabilization, *Nat Commun*, *8*, DOI: 10.1038/s41467-017-01406-6.
29. Leroy, P., S. Li, D. Jougnot, A. Revil, and Y. Wu (2017), Modelling the evolution of complex conductivity during calcite precipitation on glass beads, *Geophysical Journal International*, *209*(1), 123-140, DOI: 10.1093/gji/ggx001.
30. Li, L., et al. (2017), Expanding the role of reactive transport models in critical zone processes, *Earth-Science Reviews*, *165*, 280-301, DOI: 10.1016/j.earscirev.2016.09.001.
31. Noel, V., K. Boye, J. S. L. Pacheco, S. E. Bone, N. Janot, E. Cardarelli, K. H. Williams, and J. R. Bargar (2017), Redox Controls over the Stability of U(IV) in Floodplains of the Upper Colorado River Basin, *Environ Sci Technol*, *51*(19), 10954-10964, DOI: 10.1021/acs.est.7b02203.
32. Noel, V., K. Boye, R. K. Kukkadapu, S. Bone, J. S. L. Pacheco, E. Cardarelli, N. Janot, S. Fendorf, K. H. Williams, and J. R. Bargar (2017), Understanding controls on redox processes in floodplain sediments of the Upper Colorado River Basin, *Sci Total Environ*, *603*, 663-675, DOI: 10.1016/j.scitotenv.2017.01.109.
33. Pan, D., J. Nolan, K. H. Williams, M. J. Robbins, and K. A. Weber (2017), Abundance and Distribution of Microbial Cells and Viruses in an Alluvial Aquifer, *Frontiers in Microbiology*, *8*, DOI: 10.3389/fmicb.2017.01199.
34. Paul, B. G., et al. (2017), Retroelement-guided protein diversification abounds in vast lineages of Bacteria and Archaea, *Nature Microbiology*, *2*, 17045, DOI: 10.1038/nmicrobiol.2017.45.
35. Reinoso-Maset, E., C. I. Steefel, W. Um, J. Chorover, and P. A. O'Day (2017), Rates and mechanisms of uranyl oxyhydroxide mineral dissolution, *Geochim Cosmochim Ac*, *207*, 298-321, DOI: 10.1016/j.gca.2017.03.009.
36. Saup, C. M., K. H. Williams, L. Rodriguez-Freire, J. M. Cerrato, M. D. Johnston, and M. J. Wilkins (2017), Anoxia stimulates microbially catalyzed metal release from Animas River sediments, *Environmental Science: Processes & Impacts*, *19*(4), 578-585, DOI: 10.1039/C7EM00036G.
37. Varadharajan, C., et al. (2017), Reoxidation of Chromium(III) Products Formed under Different Biogeochemical Regimes, *Environ Sci Technol*, DOI: 10.1021/acs.est.6b06044.
38. Winnick, M. J., R. W. H. Carroll, K. H. Williams, R. M. Maxwell, W. M. Dong, and K. Maher (2017), Snowmelt controls on concentration-discharge relationships and the balance of oxidative and acid-base weathering fluxes in an alpine catchment, East River, Colorado, *Water Resour Res*, *53*(3), 2507-2523, DOI: 10.1002/2016wr019724.
39. Yabusaki, S. B., et al. (2017), Water Table Dynamics and Biogeochemical Cycling in a Shallow, Variably-Saturated Floodplain, *Environ Sci Technol*, *51*(6), 3307-3317, DOI: 10.1021/acs.est.6b04873.
40. Yuan, X., P. S. Nico, X. Huang, T. X. Liu, C. Ulrich, K. H. Williams, and J. A. Davis (2017), Production of Hydrogen Peroxide in Groundwater at Rifle, Colorado, *Environ Sci Technol*, *51*(14), 7881-7891, DOI: 10.1021/acs.est.6b04803.
41. Zaremba-Niedzwiedzka, K., et al. (2017), Asgard archaea illuminate the origin of eukaryotic cellular complexity, *Nature*, *541*(7637), 353-358, DOI: 10.1038/nature21031.

Awards

- Hubbard, S.S., named American Geophysical Union Fellow, Class of 2017, for fundamental contributions to hydrology through advancing and using geophysical methods'

Scientific Leadership and Community/DOE Service (Editorships, Scientific Advisory Boards, etc)

- Agarwal, D., Member, Canadian National Research Council Digital Technologies Peer Review
- Agarwal, D., Member, National Academies Roundtable on Data Science Education
- Agarwal, D., Participant, BERAC Subcommittee on User Research Facilities
- Agarwal, D., Member, Computing Research Association Committee on the Status of Women
- Agarwal, D., Inria International Chair, Rennes, France
- Agarwal, D., Senior Fellow, Berkeley Institute for Data Science (BIDS)
- Banfield, J., Member, Joint Genome Institute Prokaryotic Advisory Committee

- Banfield, J., selected to lead Innovative Genomics Institute Microbiology Program
- Beller, H.R., Editorial Advisory Board of CRC Press Sustainable Energy Developments series
- Beller, H.R., Editorial Advisory Board of *Environmental Science & Technology*
- Beller, H.R., Scientific Advisory Committee (SAC) for the Biosciences Division of the SLAC National Accelerator Laboratory (Menlo Park, CA)
- Bouskill, N.J., Editorial review board member for the Frontiers Journals
- Bouskill, N.J., Panel reviewer for the hydrobiogeochemistry SFA proposal submitted to DOE SBR by the team from PNNL.
- Brodie, E.L., Editorial Board: mSystems
- Brodie, E.L., Kavli Foundation collaboration to organize a cross-Berkeley (UCB/LBNL) Microbiome Initiative by the UC Vice Chancellor of Research
- Chakraborty, R., Editorial board for Frontiers in Microbio Technology
- Chakraborty, R., Chair, LBNL Women Scientists & Engineers Committee – Empowerment subcommittee
- Dafflon, B., Member, AGU Hydrogeophysics Technical Committee
- Faybishenko, B.A., Associate Editor, Geophysics.
- Faybishenko, B.A., Associate Editor, Journal of the Atmospheric Sciences.
- Faybishenko, B.A., Editorial Board, Agricultural Science and Practice
- Faybishenko, B.A., Editorial Board, Bulletin of Agrarian Sciences
- Faybishenko, B.A., Guest Editor/Academic Editor, Special Issue on Flow and Solute Transport of Journal Water
- Faybishenko, B.A., Senor Editor, Environmental Sciences, Oxford Research Encyclopedia, Oxford University Press
- Faybishenko, B.A., Principal Scientific Adviser, Institute of Water Resources and Land Reclamation, National Agricultural Academy of Sciences of Ukraine, Kiev, Ukraine
- Faybishenko, B.A., Foreign Member of the National Academy of Agricultural Sciences of Ukraine (nominated and approved by the Section on Water Resources of NAASU).
- Faybishenko, B.A., Member of Interagency Steering Committee on Multimedia Environmental Models (ISCMEM): Working Group 2 "Assessment of environmental model uncertainty and parameter estimation" and Working Group 6 "Integrated Monitoring and Modeling."
- Faybishenko, B.A., International Atomic Energy Agency (IAEA), Technical Expert and Consultant: Leader of Technical Group on Decommissioning and Remediation of the Chernobyl Cooling Pond
- Faybishenko, B.A., Technical Group Lead, Decommissioning and Remediation of the Chernobyl Cooling Pond.
- Hubbard, S.S., Co-lead, DOE-BRN water-energy report, Feb 2018
- Hubbard, S.S., Scientific Advisory Board (SAB), EPA UCB Superfund Program 'Exposome'
- Hubbard, S.S., Scientific Advisory Board, Interoperable design of extreme application software (IDEAS)
- Hubbard, S.S., Director's Council, UC Water
- Hubbard, S.S., Scientific Advisory Board, Clemson Univ EPSCoR on Fate and Transport of Radionuclides in the Environment
- Hubbard, S.S., California Council of Science and Technology (CCST) Member
- Hubbard, S.S., UCB Civil and Environmental Engineering Department Advisory Board
- Hubbard, S.S., Scientific Advisory Board, NSF Arctic Data Center
- Hubbard, S.S., Scientific Advisory Board, International Soil Modeling Consortium (ISMC)
- Hubbard, S.S., Partnership Board, ESS-Dive
- Hubbard, S.S., GSA Nominations Committee Member at Large
- Hubbard, S.S., AGU Macalwane Award Committee
- Hubbard, S.S., Executive working group, sustainable governance and funding models for CA water-data, CCST
- Hubbard S.S., Steering committee, Produced water in CA, CCST
- Karaoz, U., volunteer Science Instructor for BLAZES (Berkeley Lab Adventure Zone in Elementary Science).
- Molins Rafa, S., Associate Editor for Water Resources Research.

- Steefel, C., Associate Editor, Geochimica et Cosmochimica Acta, June 2011-present
- Steefel, C., Associate Editor, Journal of Contaminant Hydrology, 2005-present
- Tokunaga, T., Associate Editor, Water Resources Research
- Williams, K.H., Associate Editor, JGR-Biogeosciences
- Williams, K.H., Executive committee member of DOE CESD-ESS Cyberinfrastructure Working Group
- Williams, K.H., Scientific Advisory Board, SLAC Water Quality SFA (PI John Bargar, SLAC)
- Williams, K.H., Member, Board of Trustees of the Rocky Mountain Biological Laboratory
- Wainwright, H.M., IAEA Working Group on Modelling and Data for Radiological Impact Assessments II

Select Invited/Keynote presentations (partial list, 2017-present)

1. Agarwal, D., "Data Science at Berkeley Laboratory", Bureau de Recherches Géologiques et Minières (BRGM), October, 2017
2. Agarwal, D., "Data Research at LBL", NSF Macroscope Big Data Panel, November, 2017
3. Agarwal, D., "Data Science Enabling Science at Berkeley Laboratory", IBM Distinguished Lecture, November, 2017
4. Agarwal, D., C. Varadharajan, and S. Hubbard, "Moving From Information to Knowledge: Lessons from DOE Team Science", National Academies Review - Future Water Resource Needs, January, 2018
5. Banfield, J., et al., "Standing on the threshold and looking forward: incorporating microbial metabolism into understanding of biogeochemistry", Plenary 'Goldschmidt Award', Paris, France, August, 2017
6. Hubbard, S. S., "Distinguished seminar", University of Illinois, Urbana-Champain, December, 2017
7. Hubbard, S. S., "Overview of Berkeley Lab and Associated Water Research", Webinar, CA Department of Water Resources, June, 2017
8. Hubbard, S. S., "Predictive Understanding of Watershed Hydro-Biogeochemical Dynamics, enabled through the US Department of Energy Network of Watershed Testbeds", OZCAR France Critical Zone meeting, March, 2018
9. Hubbard, S. S., "Distinguished seminar", CO School of Mines, Golden, CO, April, 2018 (invited).
10. Hubbard, S. S., et al., "California Water Resiliency in an Energy Constrained and Uncertain Climate Future", American Chemical Society, Washington D.C., April, 2017
11. Hubbard, S. S., et al., "H32D-01: Predictive Understanding of Mountainous Watershed Hydro-Biogeochemical Function and Response to Perturbations", AGU Fall Meeting, New Orleans, LA, December, 2017
12. Hubbard, S.S., Beijing Normal University, Beijing China, June 2018
13. Hubbard, S.S., Tsinghua University, Beijing China June 2018
14. Hubbard, S.S., Peking University, Beijing China, June 2018
15. Hubbard, S.S., Chinese Academy of Sciences, Tibetan Plateau Research, Beijing, China June 2017
16. Hubbard, S.S., Chinese Academy of Sciences, Environmental Research, Beijing, China June 2018
17. Wainwright, H. M., "Define End-State and Optimize Monitoring Program Using High-Performance Computing Codes", IAEA MODARIA II Meeting, Brussels, July, 2017
18. Wainwright, H. M., et al, "Multiscale Data Integration for Radiation Monitoring", TERRITORIES Workshop, Madrid, Spain, June, 2018
19. Wainwright, H. M., et al, "Sustainable remediation and environmental monitoring at nuclear contaminated sites", Departmental Seminar, Tokyo University, Tokyo, Japan, April, 2018 (invited).
20. Wainwright, H. M., et al, "Multiscale Data Integration for Environmental Monitoring", Departmental Seminar, Clemson University, Clemson, SC, February, 2018
21. Williams, K. H., "Watershed Function Scientific Focus Area: Hydrobiogeochemistry from the Catchment to Basin Scale", Colorado Water Workshop, Western State Colorado University, Gunnison, CO, June, 2017

SFA members also gave > 50 contributed presentations during this performance year. Abstracts associated with SFA research at the Fall AGU are provided here: AGU booklet – 2017