

### LBNL Watershed Function SFA Annual Report 2017

#### **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. Examples of perturbations include 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, established October 1, 2016, focuses on improving predictions of mountainous watershed dynamics at 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: environmental clean-up, nutrient delivery for sustainable biofuel crops, reliable and clean water delivery, and sustainable 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



**Figure 1.** The Watershed Function SFA takes a systemwithin-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.

coupled responses to perturbations, and how responses propagate throughout the system and generate an integrated watershed discharge response, constitute a major scientific challenge.

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. The Watershed Function SFA has developed a system-ofsystems perspective, developing new methods to predict the cumulative watershed response to perturbations based on detailed information available from select subsystems within the watershed. 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 confront and exploit the hierarchical nature of natural 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, and pointed at increasing computational resources expected to be available as part of the exascale trajectory, the first-ever watershed scale-adaptive 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. Mountainous watersheds provide sixty to ninety percent of water resources worldwide, and are accordingly referred to as the 'water towers' of the world. Observational evidence suggests that mountain water resources and associated societal services 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; I T Stewart, 2009), which, along with increasing air temperature, can contribute to vegetation



**Figure 2.** The 300 km<sup>2</sup> 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.

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 project is being carried out within the East River watershed in the Upper Colorado River Basin. Among other societal benefits, the Colorado River and its tributaries supply more than 1 in 10 Americans with some, if not all, of their water for municipal use, along with irrigation water for more than 5.5 million acres of land. The basin supports more than 4,200 megawatts of electrical generating capacity, providing power to hundreds of local areas and millions of people (CRB, 2012). The

East River watershed represents a domain of  $\sim 300 \text{ km}^2$ , including both pristine and metals-impacted drainages. The watershed connects a gradient of elevation and life zones through fluid, nutrient, and sediment transport, 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) that were chosen to represent regions having expected 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 key datasets tightly coupled to models. While we are developing the SFA system-within-system 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.

Developing approaches to accurately predict watershed function and dynamics is directly aligned with the BER-CESD mission "to advance a robust predictive understanding of Earth's climate and environmental systems and to inform the development of sustainable solutions to the Nation's energy and environmental 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 through 3, which are explored in the pristine region of the watershed, although limited tasks are also underway to enable out year progress on Questions 4-6. In this limited page Annual Report, we focus primarily on describing task accomplishments associated with Questions 1 and 3 where the bulk of our FY17 efforts have been focused. The three year milestones associated with Questions 1 and 3 are provided in Figure 3.



Figure 3. Three year milestones associated with Supporting Science Questions 1 and 3.

In addition to Supporting Science Question-specific milestones, the SFA has identified crosscutting milestones (to achieve by 3, 6 and 9 years) important for addressing the Grand Challenge question. The crosscutting milestones build on and integrate across advances made through tackling the Supporting Science Questions. The overarching SFA three-year milestone, provided below, was carefully chosen for several reasons: (a) its tractability over a three-year time period, (b) to foster integration across science theme teams and supporting science questions toward a common three-year goal; and (c) to exercise the newly developed scale-aware simulation capabilities; and (4) to address an important 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 within subsystems, 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.

#### **3 ORGANIZATION**

The Watershed Function SFA team includes  $\sim$ 75 individuals, distributed across Berkeley Lab, five universities, government, and private sector companies. The project is composed of six components that represent scientific themes of the project. Component teams work together at select intensive study sites within the watershed to address the supporting science questions. The SFA organizational structure facilitates two aspects which are important for project success: (a) investigations of specific hypotheses associated with scientific themes (such as 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 are shown in Figure 4. Together with Harry Beller and Jill Banfield, this group of leads comprises the Watershed Function executive committee. Component task leads, including many early career staff, are listed below each component. Many additional team members (not shown) contribute to the identified tasks. A Scientific Advisory Board (SAB) has been assembled and engaged with the SFA; SAB members and associated expertise are described in the Appendix.



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

As described in Section 5, the project provides an integrating framework for, and benefits from, significant leveraging offered by several collaborating principle investigators and their associated staff from many institutions, who have independently funded projects affiliated with the SFA.

#### 4.0 SFA PROGRESS

The Watershed Function SFA, initiated on October 1, 2016, has realized significant progress during this reporting period. Achievements associated with select tasks, as well as overall progress toward meeting science question 3 year milestones, are described in this section. While many tasks are at an early stage, some have already led to new insights and demonstrated outcomes. Among other output this year, the SFA has produced 52 publications and given over 60 presentations, several of which were invited presentations. Of the 52 publications, 24 were published in journals with an impact factor > 5.0. A summary of the Watershed Function SFA annual products is provided in the Appendix, including journal publications, outreach, community service, invited presentations, and abstracts. The Appendix also provides information about other relevant activity or recognition, such as workshops or special session organization, awards, and relevant leadership positions during this performance year.

Figure 5 illustrates how different scientific components contribute to the supporting science questions. Cells with colored shading indicate FY17 activity, which primarily focused during this reporting period on Questions 1 and 3. We are at an early stage in the project and have not made any discoveries that could shift the SFA project to dramatically new directions. *We are awaiting news of the FY18 budgets; a decrease to the expected FY18 SFA budget could dramatically impact the project and require significant rescoping and reformulation of milestones, given the integrated nature of the project.* Due to space limitations of this annual report, we provide brief updates of select tasks only, as indicated by the tasks identified by an abbreviated name in Figure 5.

Six Supporting	Component Based FY17 Tasks					
Science Questions	Hydrology	EcoHydrology	OrganoMineral Dynamics	Watershed Characterization	Watershed Reactor	Data Management & Assimilation
Response of watershed subsytems to perturbations (hillslope and floodplain)	• Subsurface HBGC	<ul> <li>Above and below geophysics</li> <li>Vegetation</li> <li>Snowmelt BGC</li> </ul>	<ul> <li>Meander microbio</li> <li>Meander Hydrology</li> <li>Oxbow BGC</li> <li>Meander modeling</li> </ul>			
Connectivity between subsytems	• Hillslope modeling					
Aggregated watershed response			• Shale weathering	Infrastructure     Snow characteristics     Snowmelt-runoff     Vegetation stress     EMMA     Bedrock     characteristics	Snow modeling     AMR     Model development     N milestone	• DMA
Sufficient but minimum fine-scale information						
Impacted catchment responses						
Operational forecasting						

**Figure 5**. Matrix indicating specific FY17 component-based tasks and their association with supporting science questions. Colored cells indicate FY17 activity, the majority of which are associated with Questions 1 and 3. Several tasks active in FY17 are not listed; progress on tasks that are listed is provided below.

# <u>QUESTION 1</u>: 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?

#### **Intensive Site Description and Development**

In an effort to link two critical domains 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



**Figure 6.** Floodplain (left) and hillslope (right) intensive sites in the Lower Montane region of the East River Watershed.

activities at East River. The sites encompass an area of  $\sim$ 30 ha and include variations in lower montane vegetation composition (riparian and non-riparian) and fluvial morphologies, including meandering reaches, meander cutoffs, and stranded oxbows. The site is hosted on Cretaceous age Mancos shale having varying degrees of fracturing and weathering; numerous shale springs and seeps exist within the study area. The interconnected study sites enable all Components of the SFA to pursue tandem activities designed to decouple hydro-biogeochemical processes associated with both individual compartments (Q1), their aggregation (Q2/Q3), and the impact of early snowmelt via manipulation experiments planned for FY18 and beyond. Site infrastructure designed to enable this work includes the following: two stream gauging stations; stream water quality parameter sondes; automated, year

round stream sampling for water chemistry; 40+ soil sampling sites for hillslope and floodplain metagenomics; 30+ alluvial aquifer wells; two deep (10 m) hillslope groundwater wells; four boreholes instrumented for vertically resolve hydrogeochemical analysis spanning the hillslope to floodplain continuum; snowmelt monitoring and sampling; six hillslope and three floodplain ecohydrology study plots equipped with soil moisture and temperature probes; geophysical and UAV monitoring transects and flight paths; integrated meteorological station; eddy covariance flux tower. Data streams are telemetered providing real time and continuous access for QA/QC and incorporation into both hydrologic and reactive transport models describing fluid and nutrients flows within and between both compartments. All instrumentation, installation activities, and data acquisition activities (including UAV-based activities) are undertaken in accordance with USFS policies and under a USFS Special Use Permit issued to Berkeley Lab.

#### **Progress on Select Tasks**

## Hillslope subsurface water and carbon flux measurements (referred to as 'subsurface HBGC' in Figure 5)

Important segments of the hydrologic and elemental cycles reside between the soil surface and bedrock, where biogeochemical transformations are depth-distributed and coupled to the atmosphere and river via fluxes of gases, water and solutes. Thus, subsurface responses to surface perturbations need to be understood to predict baseflow and runoff exports of water and nutrients into floodplains and rivers. To gain this understanding, an integrated set of field, laboratory, and modeling studies have been initiated on a lower montane hillslope that drains into the East River. Most of the effort during this first year has focused



**Figure 7.** Cross-section illustration of the lower montane hillslope transect, showing instrumented monitoring stations.

at four monitoring stations along a 200 m hillslope transect, instrumented in 10 m deep boreholes drilled through soil into Mancos Shale. Our measurements reveal significant information about subsurface water fluxes, including infiltration/evapotranspiration dynamics within the upper 2 m of soil and saprolite, snowmelt runoff and water table rise emerging along the hillslope soil surface, and substantial baseflow through the underlying fractured Mancos Shale. Carbon inventories and fluxes from the soil surface (and seasonal in snowpack) down through fractured bedrock are being quantified through a suite of solid,

aqueous, and gas phase analyses. Subsurface respiration, sustained by organic carbon fluxes, is significant, even throughout winter. Laboratory soil and sediment analyses, microbial incubation studies, depthresolved metagenome and metatranscriptome analyses from five sites along the transect, and determination of pore water composition and fluxes are helping to develop understanding of controls on the hillslope water and carbon fluxes and their exports to the atmosphere and river. This work was presented at the GSA 2017 Annual conference.

#### Monitoring and quantifying hillslope above/below ground interactions ('above and below geophysics')

Quantifying the interactions between above and below ground properties at relevant spatiotemporal scales is critical to understand the linkages between various hydrobiogeochemical processes, their response to perturbations, and their influence on the downgradient export of water, C, N & P. We installed instrumentation and initiated investigations along the hillslope-to-hollow transect at the lower montane site. The instrumentation includes autonomous spectral cameras. soil moisture and temperature sensors and electrical resistivity tomography (ERT), sporadic measurements of canopy reflectance (ground- and UAVbased), and other datasets acquired under index inferred from the aerial image.



Figure 8. (top) Aerial image with dots indicating wells (blue), cameras (green) and vertical profiles of soil moisture sensors (red). The black line indicates the location of the ERT monitoring transect. (bottom) Comparison between soil dielectric permittivity (Kr), soil electrical conductivity (EC) extracted from the ERT top 20 cm and the greenness

different tasks (incl., biogeochemical and atmospheric data). The UAV-based aerial imaging enabled the mapping of the snow thickness distribution. UAV monitoring is currently being performed every month to monitor snowmelt and the change in plant density, shape and vigor during the growing season. Initial results reveal a strong correlation between soil dielectric and electrical properties (from ERT and point-scale data), vegetation greenness (using satellite and UAV-based data), and landscape metrics (from LiDAR data). In parallel, a multi-1D inverse modeling approach is being developed for indirect estimation of soil characteristics (incl., hydraulic conductivity) and processes (infiltration and evapotranspiration) using geophysics; this is critical as those processes cannot be easily measured directly in the field. Further statistical analysis will integrate above measurements into a machine learning algorithm to evaluate aboveand-below ground co-dynamics, the uncertainty in predicting various properties from others and the control of landscape position, soil and vegetation characteristics on the various dynamics. Results will serve to parameterize advanced biogeochemical models and to develop probabilistic mapping of soil properties at the watershed scale using UAS/aircraft/satellite-based data.

#### Gradient and Snowmelt Study Design and Early Observations ('vegetation')

We have established six new study sites across a gradient from 9,100 feet to 11,700 feet elevation (montane to alpine life zones) to determine coupled and uncoupled vegetation, soil, water processes in relation to interannual climate variation and early snowmelt manipulation. The gradient parallels long-term (since 2003) vegetation gradient study site established by SFA university collaborator Brian Enquist. By Fall 2016, we had established vegetation study plots at each site along the new gradient, which include three control and three early snowmelt at the four intermediate sites. We established common methodologies to enable comparison between new and existing sites toward quantifying how perturbations, including early snowmelt and the consequent mid-summer droughts, affect vegetation leading to changes in the export of water, C, N, and P from subsystems and the watershed.

In fall 2016, we observed many plant species re-greening, remaining green, growing new leaves and even flowering under the unusually warm fall conditions. We developed an approach to monitor these fall phenological events that were occurring at a time of year when the sites would typically have begun to accumulate snow. Our spring 2017 observations are poised at addressing if plants that grow in fall more tightly couple their spring phenology to the timing of snowmelt than species that did not grow in fall, and if so, what are the consequences? Our summer 2017 field plan includes understanding plant leaf traits, including hyperspectral characterization, for plant species that do and don't green in fall or grow rapidly following snowmelt. How does the timing and the microclimate conditions under which a leaf is produced alter plant growth and plant function throughout the growing season?

Based on the premise that greater public support and understanding of science will result from broad dissemination of the science, we are sharing the work we do in the field, our initial findings, and how these findings alter our research plans through social media as is described in the Appendix (and at @heidimountains). Our methods and early results have been presented this year to the Colorado Department of Public Health and the Environment, EPA region 8 and the Niwot Ridge LTER.

## Hillslope biogeochemical dynamics as a function of season, snowmelt and location ('snowmelt BGC')

Baseline data on hillslope biogeochemistry, particularly from snow accumulation through snowmelt periods, is being performed with a focus on microbially mediated processes (e.g., nitrification, denitrification) and with an objective to quantify the impacts of early snowmelt on export of N and C.

Over the first 6 months of the project, we have been collecting data on soil geochemistry (extractable and pore water NH<sub>4</sub><sup>+</sup>, NO<sub>3</sub><sup>-</sup>, P, amino acids) and microbiology (microbial biomass C and N and corresponding isotopic signatures; community structure based on 16S rRNA and ITS sequences; omics) as well as soil and under-snow gas fluxes and isotopic signatures. More intensive sampling is



**Figure 9.** Soil nitrate (a), ammonium (b), and microbial community composition (c) at Lower Montane site as a function of location (plot A, B, C, or Floodplain) and season (fall or winter).

occurring (and will occur) between snow accumulation and snowmelt than at other times of the year. Samples were collected along a transect from the hillslope (vegetation plots A, B, C) to the floodplain. The clearest trends to date have indicated that the floodplain plots, which have higher water content than the hillslope plots, have lower nitrate and higher ammonium concentrations than the hillslope (Fig. 9), at least partly as a function of redox state (i.e., more reducing conditions). Soil microbial communities (analysed for bacteria and archaea so far, fungal sequencing underway) indicate that location (floodplain vs. hillslope) is more differentiating among samples than season (fall vs. winter) or specific hillslope location (i.e., A, B, or C plots) (Fig. 9).

## Surface-subsurface hydro-biogeochemical simulations along the hillslope intensive site ('hillslope modeling')

While many studies of hillslope hydrology have provided predictions on how aspects of systems respond to warming and disturbance, hydrologic and biogeochemical changes remain uncertain, as do their contribution to overall watershed function. 2-D (x-z) models are being used to investigate the primary

controls on water, energy, and carbon fluxes along the intensive hillslope transect within the East River Watershed.

To understand the impact of subsurface heterogeneity on the water-energy balance, a series of numerical experiments with the integrated hydrologic model ParFlow were conducted. Ensembles of geostistical random fields of subsurface heterogeneity composed of 50 realizations each were generated at differing variances of hydraulic conductivity  $(\ln(K)=1 \text{ m/hr and } \ln(K)=10$ m/hr). Correlations between yearly averaged latent heat flux and water table depth for both hydraulic conductivity ensembles show nearly identical mean behavior at shallow water table depths (<2 m) but weaker correlations as subsurface heterogeneity increases. The breakdown of the land to subsurface connection with greater subsurface heterogeneity is a new finding obtained from this study. In order to further establish linkages between surface and subsurface hydrologic and biogeochemical components, future efforts will focus on integrating ParFlow surface flow components into the flow and reactive transport code TOUGHREACT under steady and punctuated flow conditions.



We also examined the impact of warming using long-term (1979– 2010) climate data and run a comprehensive mathematical process snowpack accumulation and nitrogen dynamics model, ecosys to study the impacts of ambient versus warm

Figure 10. ecosys simulations show differences in under ambient and 1 degree warmer conditions.

conditions on snowpack, biogeochemical processes and gross primary productivity (GPP) (Fig. 10). Model results show that warming advances snowmelt by 26 days (Fig. 10a) which is close to the advancing ambient snowmelt rate proposed by Harte et al. (2015) at 0.74 days/year  $\approx$  22.2 days. We further quantified the impact of this earlier snowmelt on nitrogen dynamics at the site. These preliminary results indicate that warming may enhance N mineralization under snow, and combined with earlier snowmelt may result in earlier and greater nitrate release (Fig. 10b). A continued shrub expansion was predicted with corresponding increases in GPP (Table 1) in the absence of drought

TABLE 1	GPP under normal weather conditions (gC/m²/year)	GPP under 1 degree warmer conditions (gC/m <sup>2</sup> /year)
Sedge (forb)	62.74	82.63
Broad leaf (shrub)	63.40	221.53
Ecosystem total	126.35	304.69

#### Characterization of microbial diversity and function in meander-associated floodplain intensive site using genome-resolved metagenomics ('Meander Microbio')

Meander-associated riparian zones (MARZs) are subject to natural perturbation events (*i.e.*, flooding, water table level change, and hillslope runoff) that connect soil microbial communities to the rest of the watershed. Our approach to expanding understanding of the role of MARZ soil microorganisms in biogeochemical cycling to the watershed scale was to target discrete meandering reaches of the East River (ER) as a potentially representative repeating motif. 94 soil samples were collected over the  $\sim$  10-25 cm depth interval from three meandering reaches: upstream (ERMG), midstream (ERML), and downstream (ERMZ). DNA sequence information from individual samples was processed and assembled using standard methods. 184 near- complete draft genomes, representing 94 different organisms have been recovered to this point through ggKbase binning. Betaproteobacteria are the most abundant members of the microbial community in all three MARZs, and they are mostly affiliated with other Betaproteobacteria previously only seen at the Rifle site. Rank abundance curves of the most abundant groups (Fig. 11) show that the same groups of

Betaproteobacteria are commonly found among all three MARZs, supporting the idea that these subsystems could be used as scaling motifs in modeling ecosystem functioning. Furthermore, many of these Betaproteobacteria have the potential for sulfur oxidation, suggesting that this process may be relevant at the watershed scale and deserves further investigation. Our preliminary findings have been presented at the 12<sup>th</sup> Annual DOE Joint Genome Institute Genomics of Energy & Environment Meeting.

Figure 11. Rank abundance curves for organisms with median abundance  $\geq 2$  based on rpS3 (corrected by sequencing depth across all samples). Average abundance across all samples from each meander and 95% confidence intervals are shown. Abundant groups of bacteria shared among all three meanders indicated with asterisks. Groups shared between ERMG and ERML are indicated with downward pointing arrows. Groups shared between ERML and ERMZ are indicated with upside down triangles.

#### Interactions between floodplain meander geomorphology, stratigraphy and dynamic hydrology as controls on surfaceground water (SW-GW) exchange ('Meander Hydrology')

This task strives to fill key science gaps related water-floodplain interaction, including improving: 1) the representation of meander geomorphology and sedimentology and 2) the inclusion of dynamic, snowmelt-dominated hydrology in watershed-scale models of SW-GW exchange in the floodplain. Improved system representation within models and field experiments facilitate simulation of various snowmelt scenarios and evaluation of impacts on SW-GW exchange across the watershed's floodplain. Buried fluvial sediment packages (former channels and alternate bars) comprise floodplain sedimentology, exhibit contrasting hydraulic conductivities and dimensions, and affect the length and timing of SW-GW exchange. To improve estimates of fluvial complexity in watershed-scale models of SW-GW exchange, we developed a novel approach of mapping fluvial stratigraphy across multiple scales that combines point descriptions of floodplain sediments, ground penetrating radar (GPR) surveys, and remote sensing techniques. The East River is actively meandering, allowing for observable connections between floodplain evolution and resulting sedimentology, and subsequently, the use of remote sensing approaches to estimate the location of key sediment packages across the watershed's floodplain.

We additionally found that surface discharge and groundwater conditions in the East River vary strongly between spring snowmelt and baseflow (Fig. 12). Field observations and preliminary results from tracer tests suggest that these contrasting conditions influence where and how fast surface water moves laterally across the meander by affecting surface flow geometry and in which fluvial sediment packages the exchange occurs. In order to estimate the impact of changing snow-melt additional



River Discharge Water Year 2016



**Figure 12.** River discharge (courtesy of R. Carroll), groundwater elevations, and piezometric gradient (inset) at Meander D at the pumphouse field site. Surface and groundwater conditions vary strongly between spring snowmelt and baseflow.

field experiments are needed to measure the interactions between contrasting hydrologic conditions and the floodplain system.

The activity results were presented at the 2016 AGU and GSA conferences and are the result of collaboration between students and scientists at the Colorado School of Mines, LANL, LBNL, and Colorado College. The results of the GPR and remote sensing work are currently in preparation as a manuscript for the Earth Surface Land Processes Journal.

#### Meander and Oxbow biogeochemistry ('Oxbow BGC')

The overarching goals of this task are to: identify and quantify the important biogeochemical processes in the soils and sediments of active meanders and meander cutoffs (oxbows) that lead to release and uptake of metals, nutrients, and carbon; to compare how these processes change when an active meander is cut off; and to determine how both systems respond to hydrological perturbations.

Sediment core and water samples were taken from Meander C and Meander O, Meander C being an active floodplain meander and Meander O being a recent oxbow cutoff with similar gross morphology to Meander C, Figure 13. The water chemistry, collected from a transect of piezometers across Meander C showed a distinct and stable under low water conditions, year over year and month over month,



**Figure 13.** Piezometer (red and green) and core (yellow) locations across the current active Meander C transect and the comparable recent Meander O cut-off.

redox gradient with pronounced decreases in dissovled oxygen and corresponding increases in dissolved Fe(II) and dissolved organic carbon near the center of the transect. Other redox active species such as uranium also showed redox driven changes in concentration. In the case of uranium this led to pore water concentrations lower than river water due to its decreased solubility under reducing conditions, indicating potential uptake by the sediments. The texture characteristics also varied with position across the transect with the finest grained material in the center of the meander and corresponding to the most reducing conditions. The fine-grained sediment in the center of Meander C also had the highest levels of organic carbon and extractable Fe(II). In contrast, the transect across the Meander O cut-off showed the opposite trend in which the highest dissolved oxygen was found in the center of the meander and corresponded with the minimum Fe(II) and maxium dissoved uranium. These results support the hypothesis that redox processes within floodplain features can lead to the release (e.g. organic carbon) or uptake (e.g. uranium) of important chemical species and therefore impact the chemistry of the river and the eventual export of these species. They also support the hypothesis that changes in river morphology through the formation of cut-off meanders may dramatically alter the biogeochemical conditions in large volumes of sediment within the floodplain, potentially impacting export of carbon, metals, and nutrients from the system.

The results from this task were used to calibrate and challenge the meander modelling activities presented in the next section. Further investigations will determine how hydrologic perturbations, like spring peak flow, impact the redox gradients within these features and the export of chemical species to the river.

#### Meander/Hyporheic Modeling ('Meander modeling')

The overarching goal of the meander/hyporheic modeling task is to understand hydrological and biogeochemical processes through hyporheic zones consisting of riverbeds, meanders, and floodplains to develop a predictive capability for C, N, P dynamics at the watershed scale. The hypothesis is that biogeochemical gradients that exist within the hyporheic zone significantly impact carbon and nutrient fluxes in the larger East River system, particularly when upscaled over the entire length of the East River Flood Plain. Joint river and hyporheic zone controls on aquatic respiration and denitrification are estimated

to be disproportionately large relative to their size, yet the physical factors impacting their function confound an integrated ecosystem interpretation. To test how these "integrator" zones influence redox chemistry in response to various scenarios of early snowmelt and summer storm frequency, we developed a zero order mass balance model for the river coupled to subsurface flow and reactive transport models to represent the hyporheic zone. Additionally, the aggregated functioning of two active meanders was explored using PFLOTRAN. A complex reaction network was integrated into the zero order/hyporheic coupling and PFLOTRAN models that included a full redox sequence and biotic and abiotic processes to model biogeochemical zonation within the hyporheic region. Perturbations were included through transient boundary conditions to represent the snowmelt baseflow control on flow to the river and storm control on the river hydrograph.



Figure 14. A complex reaction network incorporated abiotic reactions, aqueous speciation, mineral precipitation/dissolution reactions, microbially mediated redox reactions, and heterotrophic and chemolithoautotrophic pathways.

Simulation results using the zero order model showed that

coupled biological, microbial, and physical processes at river beds influence critical ecosystem services such as net ecosystem productivity. Our findings also revealed strong snowmelt controls on gaseous C and N loss through floodplains and hyporheic zones to the atmosphere. Additionally, springtime snowmelt strengthened river autotrophy while supporting greater summer denitrification suggesting strong shifts toward net C and N storage. The three-dimensional model in PFLOTRAN was able to predict the hydrological and biogeochemical fluxes in the subsurface. In particular, simulation results, consistent with observations, showed that nitrate, dissolved oxygen, and dissolved organic carbon values decreased, while iron (Fe (II)) concentrations increased along the meander centerline transect with distance from the stream. Results also demonstrated that hyporheic flow paths and sinuosity significantly impacted carbon and nitrogen export into the stream system. Results were presented at the AGU 2016 conference, and are in preparation to the journal Ecosystems and Water Resources Research. Key collaborators include Mike Wilkins, Audrey Sawyer, and Jonathan Raberg.

#### SUMMARY OF SELECT PROGRESS TOWARD QUESTION 1 THREE YEAR MILESTONES:

The above task summaries document several direct contributions to the Question 1 Three Year Milestones provided in Figure 3. Select examples include:

- Established and heavily instrumented two lower montane SFA intensive sites as well as observation stations along an elevation-dependent vegetation gradient.
- At the hillslope site:
  - Documented seasonal subsurface water dynamics, including infiltration/evapotranspiration dynamics within the upper 2 m of soil and saprolite, snowmelt runoff and water table rise emerging along the hillslope soil surface, and substantial baseflow.
  - Used ParFLOW numerical experiments to document how latent heart flux varies as a function of water table depth and subsurface heterogeneity.
  - Discovered that subsurface respiration, sustained by organic carbon fluxes, is significant, even through the winter.
- At the floodplain intensive site:
  - Used tracer tests and geophysics to document that surface discharge and groundwater conditions in the East River vary strongly between spring snowmelt and baseflow, and that river stage influences where and how fast surface water moves laterally across meanders;
  - Documented spatial variability of geochemical constituents, such as dissolved Fe, as a function of meander geomorphology;

- Used genome-resolved metagenomics to document the spatial variability in microbial ecology at floodplain intensive site, which is important for developing a 'meander scaling' strategy. Study also revealed the abundance of Betaproteobacteria and affiliations that were previously only identified at the Rifle Site;
- Developed and used PFLOTRAN coupled to reaction networks to simulate hyporheic zone processes, revealing: strong coupling between biological, microbial, and physical processes in riverbeds that influenced net ecosystem productivity; strong snowmelt controls on gaseous C and N loss to the atmosphere through floodplains and hyporheic zones; and that springtime snowmelt strengthened river autotrophy while supporting greater summer denitrification, suggesting strong shifts toward net C and N storage
- Documented that the location (floodplain vs. hillslope) has more of an influence on microbial ecology than does the season (fall vs. winter).
- Used *ecosys* to numerically explore the impacts of ambient versus warm conditions on snowpack, biogeochemical processes and gross primary productivity (GPP) at the 'Harte' long-term warming study site. Model results of snowmelt timing related to temperatures agreed well with previous longterm observations, and indicated that warming may enhance N mineralization under snow, potentially resulting in earlier and greater nitrate release.

#### QUESTION 2: How do interactions between vegetation, hydrology, subsurface biogeochemistry and geology, particularly in response to perturbations, vary along diverse watershed gradients and contributed to aggregated C, N, P and metal exports from the watershed?

Tasks associated with this science question strive to gain an understanding of distributed watershed properties and processes, and how those aggregate to vield an integrated watershed concentrationdischarge signature.

#### **Progress on Select Tasks**

#### Watershed infrastructure (referred to as **'Infrastructure' in Figure 5)**

Upgrades and improvements to site infrastructure at Berkeley Lab's East River study site focused on Figure 15. Schematic representation of fluxes emanating from expanding the network of stream gaging stations, deep groundwater wells, and hillslope, floodplain,



different subsystems in the watershed, and their contribution to an aggregated downgradient signature.

and stream water sampling and monitoring equipment. Upgrades to the six existing meteorological stations included a new satellite based telemetry system and sensor adjustments designed to improve the sensitivity to snow depth and soil moisture. Installation of a seventh meteorological station occurred at the SFA's intensive hillslope study site, as did installation of an Eddy Covariance flux tower at the intensive floodplain study site in collaboration with University partners (Section 5). A stream gaging station was established on Oh-Be-Joyful Creek to enable development of concentration-discharge relationships for one of the principle metal-impacted drainages in the watershed; a gaging station was also installed on Washington Gulch to provide better constraint on discharge within the primary drainage hosting the ecohydrology satellite study sites. Stream sampling activities within the metal-impacted Coal Creek drainage were greatly improved by the installation of an auto-sampler collecting samples at 2-day intervals. Four 10 m deep boreholes were drilled along the intensive hillslope study site to recover samples spanning the soil to bedrock profile, with vertically resolved pore water and soil gas samplers installed along with soil moisture, matric potential, and temperature probes. Two monitoring wells were installed for bedrock aquifer fluid sampling and to record

seasonal variations in groundwater elevation and fluid conductivity. Similar sampling equipment was emplaced over the 1.5 m depth profile on the floodplain adjoining the hillslope study site. Equipment for continuous monitoring of stream bed temperature and redox conditions over 1m depth profiles was installed in collaboration with University partners (Section 5).

### Observing and modeling snow processes across spatial and temporal scales ('Snow Characteristics' and 'Snow Modeling')



**Figure 16.** Multi-year comparison of ParFlow-CLM derived estimates of SWE with direct measurements made at the Niwot Ridge, Colorado SNOTEL station.



**Figure 17.** LiDAR derived estimate of snow depths in the East River watershed on April 2-3, 2016

Changing climatic conditions and climate perturbations are challenging our conceptualization of processes that govern snow accumulation and melt over seasonal to decadal timeframes, with studies performed at the East River study addressing these challenges through linked site observational and modeling studies spanning scales from individual subsystems to the aggregated watershed. Recent work has found that snow formulations in physically-based land surface models perform poorly in the Rocky Mountains; a finding attributable to complex terrain and vegetation heterogeneity that are insufficiently resolved at coarser scales. We combined modeling with airborne and ground snow data to validate the land surface model in ParFlow-CLM at locations having co-located meteorological and snow observations to understand parameters driving precipitation partitioning, sublimation, and snowmelt. Hourly simulations were run over multiple years to evaluate model performance at high temporal resolution and to explore the effects of altered precipitation patterns with climate change. To better understand snow accumulation and melt in complex terrain and within and between watershed subsystems, the land surface model was applied to the ~300 km<sup>2</sup> East River study domain. Model outputs were interpreted using LiDAR data collected during snowfree and snow-covered times of the year, with data used to generate estimates of snow depth, snow water equivalent (SWE), snow albedo, and radiative forcing from dust.

Remote observations of snow properties were complemented by ground sampling to improve estimates of snow density and SWE and to quantify uncertainty in model derived estimates. Ground sampling was used to quantify variations in snow pack water isotope composition as a function of elevation, aspect, and predominant vegetation

type, with the isotope data serving as an important constraint on seasonally dependent contributions of snow melt to streamflow and groundwater recharge. The combination of point-scale observations with high resolution modeling and airborne data is providing new insight into snow processes from the individual subsystem (e.g. montane hillslope) to the watershed scale. This combined approach uses modeling to bridge the gap between spatial and temporal limitations of direct measurements and observations. In turn, observations build confidence that physical processes important to snow accumulation and melt are adequately captured by models.

Findings were presented at the 2016 AGU conference and are in preparation for submittal to *Environmental Modeling and Software*. Remote data collection was performed in close partnership with NASA/JPL's

Airborne Snow Observatory team. The linked model-data approach constitutes an early demonstration of improved data assimilation approaches needed to quantifying fluxes of water, nutrients, and metals over operationally relevant scales.

#### Snowmelt-runoff analysis ('Snowmelt-runoff')

Snowmelt is an important water resource and vital to ecosystem functioning particularly in the Western US. In this task, we aimed to identify and quantify the effect of increasing temperature on snow and streamflow dynamics using historical data. A statistical data mining approach was used to decouple the effects of precipitation and temperature by exploiting their inter-annual variability. The Kendal rank-correlation test confirmed that the quarterly average temperature has a significant upward trend of  $1.0-1.9^{\circ}$  C per decade. Despite increasing temperature, the snow and streamflow metrics – peak snow water equivalent (SWE), snowmelt timing (e.g., onset of melting, first bare-ground date), peak flow rate and timing, annual total discharge – did not show any significant trends due to the large inter-annual variability in winter precipitation. The correlation and principle component analysis, however, identified the effect of spring temperature on those metrics, depending on different seasons.

We found that (1) winter precipitation primarily influences the peak SWE and annual total discharge, while spring precipitation affects the timing of melting and peak flow, (2) increasing spring temperature not only shifts the peak flow earlier but also reduces and broadens the peak flow and reduces annual total discharge, and (3) the summer monsoon precipitation does not significantly contribute to the annual discharge. We also used a regression analysis and a Lindeman-Merenda-Gold importance metric to quantify the temperature effect. We found that that monthly temperature in spring explains the variability of the first snow-free date by the equivalent standard deviation of 3.4-4.4 days, and the total discharge by 10–11%.

analysis Our also suggested that increasing winter temperature would start affecting peak SWE in this region this decade. potentially leading to significant changes in snowmelt timing and streamflow, and we should expect to see a significant change in snowmelt timing and streamflow. The activity results were described in the paper submitted to Geophysical Research Letters.



**Figure 18.** Biplots of the first and second principle components (PC1 and PC2): (a) snow and snowmelt-related variables, and (b) streamflow-related variables. The snow and streamflow variables are indicated by red (total Q as total annual discharge), while other variables are in black (T as temperature and P as precipitation).

#### Vegetation

#### Characterization and Stress Response ('Vegetation Stress')

Plant functional types and their dynamics have a significant control on soil biogeochemical properties and also water budget through evapotranspiration. At the same time, subsurface biogeochemical and hydrological processes have a large influence on plant traits and dynamics so that plant characteristics and dynamics can be considered as "surface expressions" of subsurface processes. This task lays the framework to explore a "plant as soil sensors" concept, which we believe will be a powerful tool to identify and quantify subsurface heterogeneity based on the co-variability with plants.

To characterize the heterogeneous plant functional types (PFTs), we developed a data-fusion framework to integrate high-resolution satellite images and LiDAR plant heights. We demonstrated our approach at the lower montane hillslope and confirmed that our method can estimate the spatial distribution of plant functional types more accurately than currently available maps (Fig. 19). The distributed PFT map was used to parameterize the hillslope-scale ecohydrological model. We also explored the co-variability between plant functional types and subsurface properties obtained from geophysics (e.g., surface electrical resistivity tomography). We found the strong co-variability; for example, shrubs are more abundant in lithologies that facilitate drainage and are thus drier.

The stress response of plants to droughts was mapped based on the historical satellite and metrological datasets. We first define the drought sensitivity – as a scalable metric – based on annual peak NDVI (Landsat 5) and Palmer drought index, following the plot-scale studies. Non-parametric tree-based machine learning methods were used to identify the significant environmental controls on the drought sensitivity.



Results show that the drought sensitivity is negatively correlated with elevation, suggesting the increased water limitation in lower elevation due to less snow and higher temperature. The drought sensitivity is more spatially variable in shallow-rooted plant types (such as grassland), affected by local hydrological conditions. In addition, we found geomorphological and geological controls, such as high drought sensitivity in the well-drained glacial moraine regions with larger slopes. Our results were presented at the 2016 AGU conference.

Figure 19 Estimation of plant functional types in lower montane regions

#### End-Member Mixing Analysis to Identify Seasonal Stream Sources ('EMMA')

End-member mixing analysis (EMMA) was developed for the East River, CO using a suite of natural chemical and isotopic observations. EMMA is an initial step to elucidate source contributions to streamflow and address scalability and applicability of mixing processes and export of solutes in a complex, highly heterogeneous, snow-dominated catchment.

EMMA relies on principal component analysis to reduce the number of dimensions of variability (U-space) for use in hydrograph separation. The mixing model was developed for the furthest downstream and most heavily characterized stream gauge in the study site (PH). Potential tracers were identified from PH discharge as near linear (Mg, Ca, Sr, U. S SO<sub>4</sub>, DIC,  $\delta^2$ H and  $\delta^{18}$ O) with alternative groupings evaluated. The best model was able to describe 97% of the tracer variance in 2-dimensions with low error and lack of residual structure. U-space positioning (Fig. 20) resulted in seasonal stream water source contributions of rain (9-16%), snow (48-74%) and groundwater (18-34%). EMMA developed for PH did not scale across 10 nested subcatchments. Differences in mixing ratios are likely attributable to, (1) biogeochemical processes of sulfate reduction in the floodplain sediments; (2) source rock contributions from Mancos Shale and Morison Fm; (3)



**Figure 20.** PH stream water and end-members projected into U-space for baseflow (b), rising (r), falling (f) & monsoon (m) components of hydrograph.

hydrologic partitioning induced by feedbacks within the critical zone; and (4) associated subsurface flow paths. A manuscript describing the EMMA study is in preparation for Hydrology and Earth Systems Sciences and it is anticipated findings will be given at the 2017 fall AGU meeting.

#### Bedrock geophysical characterization ('bedrock characteristics')

Determining soil and bedrock characteristics is critical for understanding flowpaths, relative amounts, residence time and geochemistry of water within the East River system and for predicting how the interaction between different watershed compartments will respond to dynamic perturbations (incl. drought and early snowmelt) and influence downgradient export of water, C, N, & P. In this task, the mapping of the spatial distribution of subsurface properties in the watershed is done by integrating electrical resistivity tomography (ERT) and seismic surveys, remote sensing data (LiDAR and airborne) and wellbore and geological information. Results show that the Cretaceous Mancos Shale, which is the primary Watershed bedrock, is spatially quite heterogeneous, with alteration patterns possibly influenced by igneous dikes, initial mineralogical composition, topographic stress, preferential flow paths and river channel evolution. The bedrock Shale located in and upstream of Gothic tends to be more competent. Also, the bedrock tends to be more competent under the river bed than under the surrounding hillslopes. Data mining will be used



**Figure 21.** ERT and seismic transects at the Lower Montane site. Black intervals on the ERT represent shale identified during drilling. ERT indicates that fracture density (or shale weathering) is highest in the upper part of the hillslope. Seismic refraction tomography shows that the depth to more competent shale (bottom black line) is correlated with change in slope and consistent with the dip on the geological map.

to quantify these relationships and use them with large-scale remote sensing datasets to distribute estimates of bedrock characteristics throughout the watershed. This work will be combined with other tasks related water/soil/rock to geochemical composition and isotopic signatures. Also, external collaboration has been initiated with Burke Minsley (USGS) who will lead an airborne electromagnetic, magnetic and radiometric survey over the entire watershed.

#### Shale Weathering ('shale weathering')

Studies of shale weathering will constrain the mechanisms and rates of release of nutrients and contaminant

metals to the watershed and provide the means to gauge the effect of shale weathering on the biogeochemistry of the watershed.

We acquired grab samples, hand-drilled cores and one 10 m drill core of Mancos shale from sites throughout the watershed and analyzed them for elemental composition, isotopic and mineral analysis. Mancos shale contains numerous metals such as U, As, Re, Se, Cd, Cu and Mo that are enriched (relative to average crust concentrations) and that are lost by weathering. Several transition metals including Zn and Cd are present as sulfide minerals that are susceptible to oxidation. Using X-ray CT scans from the Energy Geosciences Rock Imaging Laboratory, we identified various features of the shale cores, including fractures centered on weathered zones. Preliminary analysis of natural fracture surfaces in rock cores indicates highly variable weathering rates in subsurface zones



**Figure 22**. Sulfur concentration *vs.*  $\delta^{34}$ S comparing weathered and unweathered shale samples. The dashed line represents the  $\delta^{34}$ S of a coarse pyrite samples, the purple band represents the  $\delta^{34}$ S of shale-affected groundwater

beneath soil and in outcrops above the water table. Weathering causes a loss of S, reflecting oxidation of pyrite, accompanied by a trend towards heavier  $d^{34}S$ . Fine-grained early diagenetic pyrite with light  $\delta^{34}S$  is preferentially weathered relative to coarser pyrite with heavier  $\delta^{34}S$  (Fig. 22). The carbonate fraction of shale samples has relatively low <sup>87</sup>Sr/<sup>86</sup>Sr, while the residual fraction has very high <sup>87</sup>Sr/<sup>86</sup>Sr. Both these signatures may provide indices for weathering that are transferred to ground- and surface water. Shale groundwater collected from wells in the Hillslope transect contains metals likely derived from shale weathering. High variability in the concentrations of redox sensitive metals and in <sup>87</sup>Sr/<sup>86</sup>Sr with depth indicates the presence of fracture networks with different water sources and biogeochemical (redox) conditions. Redox variability is also reflected in  $\delta^{238}$ U of groundwater, indicating local reduction of U.

#### An embedded-boundary adaptive mesh refinement watershed simulator ('AMR')

Accurately capturing gradients is critical to quantifying water and C, N, and P fluxes in watersheds. Adaptive mesh refinement is a numerical technique for adjusting the resolution of computational grids near important features to enable more accurate calculations locally, providing a multi-resolution approach to solving multiscale watershed processes.

We have developed a surface-subsurface solver based on the kinematic wave and Richards equations based

on the software package Chombo. Chombo provides tools for the solution of partial differential equations in Cartesian grids using the embedded boundary method to capture complex geometries and the adaptive mesh refinement approach to accurately resolve processes in focused areas of the domain (e.g., Figure 23). One of the main challenges in the simulation of integrated hydrology processes is the coupling between overland surface and groundwater flow. In our approach, the embedded boundary method is used to describe the surface topography of the watershed and provides the connection between the surface and subsurface flow problems. Adaptive mesh refinement (AMR) is a numerical technique for adjusting the resolution of computational grids near important features to enable more accurate calculations locally, and to reduce the computational burden of large domains.



**Figure 23.** Close-up view of AMR levels used to capture steep surface topography areas in a section of the East River Watershed.

As part of Chombo, AMR is useful in the integrated hydrology model in accurately capturing water fluxes that develop in localized areas of the simulation domain, such as where surface gradients are steep. A manuscript summarizing the embedded-boundary method to couple surface-subsurface hydrology is in preparation. Further, AMR is being brought to bear on a code benchmarking exercise also involving Parflow and ATS/Amanzi.

#### Trait and vegetation module development and benchmarking ('Model development')

Accurate models are needed to capture the interactions between vegetation, hydrology, microbiology and their impact on C, N, P exports from the watershed.

We are developing an approach to add vegetation models into hydrological codes (e.g. ATS, ParFlow) in order to account for water, carbon, nitrogen cycling. In particular, we are incorporating nutrient cycling and uptake by plants into hydrology codes and improve on the representation of PFT's. The approach entails the development of a *generic* code interface, i.e. an interface that is not tied to any one code.

To address the need for a better representation of microbially mediated processes in hydrological models, a framework is under development that allows for the automatic conversion of 'omics data directly into reaction networks. This network is driven by microbes and encompass any significant trait linkages observed in the data. The model environment can therefore be tailored specifically towards an environment of interest.

A great portion of this task entails code development, which is being managed using software versioning and a shared repository. The product of this work will be made available via an open-source license.



Figure 24. (Left) Schematic of vegetation role in hydrology models. *Modified after Condon and Maxwell, 2015*. (Right) Framework for building reaction networks from metagenomic datasets.

#### Nitrogen Milestone ('N milestone')

As was described in Section 2, the nitrogen milestone is an overarching SFA three year milestone, focused on evaluating the hydrological controls on the sources and sinks of nitrogen across a mountainous watershed composed of heterogeneous hot spots within subsystems, coupled to the modeling goal of 'using scale-adaptive approaches to represent the feedback between hydrological perturbation and above-and belowground biogeochemical processes to improve predictions of nitrogen export from the catchment'.

The nitrogen milestone characterizes the sources and sinks of nitrogen across different sites in East River catchment. The milestone attempts to account for the magnitude of different sources of nitrogen (Fig. 25), the cycling of different nitrogen specific following the Damköhler approach, and the form and magnitude of nitrogen export from that subsystem.



**Figure 25.** Hypothetical box mode for characterizing the nitrogen cycle and its budget across distinct regions of the watershed.

The Nitrogen Task has focused during this performance period across both intensive SFA sites (the lower montane hillslope-floodplain transect) as well as specific satellite sites of contrasting vegetation, geomorphology, soil texture and river nitrate fluxes. Recent work has shown nitrate export fluxes from East River tributaries to span two orders of magnitude and show a chemodynamic relationship with discharge. The controls on this chemodynamic behavior, and the magnitude of gaseous losses from hotspots across the watershed, are critical gaps in our knowledge that prevent a coherent N-budget being developed. The N-milestone will use extensive fieldwork during 2017 to bridge the gaps in our current knowledge.

#### Data Management and Assimilation ('DMA')

Many significant data management capabilities were developed this year that provided improvements to the data accessibility and quality, including: automated processing of and access to weather station data; a community watershed interactive portal providing information about the study sites, experiments, and data collected; QA/QC processing of the data; a data access portal; and a data package system.

Many new data streams from the East River watershed were automated and added to the online BASIN-3D SFA data management portal. These stations include: 6 weather stations, CSM weather station, NRCS SNOTEL, EPA castnet station, weather underground stations, instrumented wells in the floodplain, geochemical samples, and analytes. An updated version of the BASIN-3D software was released with improved search and data plotting capabilities. A data package system was also implemented to provide support for archiving of Watershed SFA data.



The new community watershed interactive portal described in the SFA proposal response to review



document was implemented and released this year. The interactive map identifies sites where the SFA team and collaborators are acquiring different types of measurements within the watershed.

QA/QC of time series data including meteorological data was implemented to enable outlier detection and removal as well as gap-filling. The automation also computes aggregates needed by modelers. We have also developed and posted the SFA data policy:

https://drive.google.com/file/d/0Bz9Zv4YIp0kPVnpZTkRNb0ZyQ2tTdEFZX0xwc05QX0VzRDFj/view

A range of diverse datasets have been entered into the SFA database, including:

- 2731 aq geochemical samples from 28 locations with more than 70000 analyte/location pairs
- More than 5 million time, data pairs from instrumented sensors from over 50 locations (both from direct SFA funded and collaborators). Note that some stations have four data points for each time and others have fifteen data points, so probably more than 30 million time, value pairs
- 28448 x 39816 Lidar elevation data (exposed through API)

#### **PROGRESS TOWARD QUESTION 3 THREE YEAR MILESTONES**

The task summaries provided above document several direct contributions to Question 3 Three-Year Milestones (provided in Figure 3), including:

- Developed and tested a linked model-data approach for providing new insight into snow accumulation and snowmelt physical processes in complex terrain, over scales ranging from the individual hillslope intensive site to the 300 km<sup>2</sup> watershed, using airborne and ground based measurements and ParFLOW-CLM.
- Data mining approach used with historical precipitation-streamflow discharge data to discover that winter precipitation primarily influences the peak SWE and annual total discharge, while spring precipitation affects the timing of melting and peak flow and that summer monsoon precipitation does not significantly contribute to the annual discharge.
- End member mixing analysis of downgradient stream water, performed using chemical and isotopic fingerprinting, revealed seasonal stream water source contributions from rain, snow and groundwater.
- Developed a new fusion approach, and used it to quantify plant functional types, their co-variability with subsurface geology and other variables, and susceptibility to drought stress. Discovered that subsurface lithology exerts control on PFT and that drought sensitivity is negatively correlated with elevation, suggesting the increased water limitation in lower elevation due to less snow and higher temperature.

- Developing an understanding of the geophysical signature of Mancos Shale bedrock characteristics and associated spatial variability
- Identified natural fracture surfaces in Mancos Shale rock cores from various locations in the Watershed, indicating highly variable weathering rates in subsurface zones beneath soil and in outcrops above the water table, which reflects oxidation pyrite that leads to a loss of S.
- To overcome obstacles associated with coupling overland surface and groundwater flow development, used an embedded boundary method to describe the surface topography of the watershed and the connection between the surface and subsurface flow problems. As part of the scale-adaptive model development, used Adaptive mesh refinement (AMR) to adjust the resolution of computational grids near important features to enable more accurate calculations locally, and to reduce the computational burden of large domains.
- Discovered that nitrate export fluxes from East River tributaries to span two orders of magnitude and show a chemodynamic relationship with discharge.
- Developed a community watershed interactive portal providing information about the study sites, experiments and data collected

#### APPENDIX I

#### 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.

- John Bargar (SLAC): Sampling of organic matter-rich transient reduced zone sediments along the Slate and East River drainages in support of SLAC's "Groundwater Quality" SFA renewal proposal.
- 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. Distributed temperature sensing data collected along the East River to identify putative regions of groundwater discharge.
- **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.
- Scott Fendorf (Stanford): 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.
- Li Li (PSU): Data mining and development of a reactive transport model 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.
- 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 to be assimilated into larger SFA modelling effort.
- **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).
- **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.

- 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.
- 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.
- Neslihan Tas (LBNL): Quantifying seasonal variations in microbial community composition and functionality through metagenomics analysis of riverine samples collected within the East River drainage.
- **Rich Wanty** (USGS): Identification of deep groundwater controls on metals release from subcatchments within the Slate River drainage through collection of hydrogeochemical data and precursory geophysical information in support of planned drilling and watershed-scale airborne electromagnetic survey activities.
- Mike Wilkins (OSU): 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.

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- Manning, A. H., P. L. Verplanck, J. S. Caine, and A. S. Todd (2013), Links between climate change, water-table depth, and water chemistry in a mineralized mountain watershed, *Appl Geochem*, 37, 64-78, DOI: 10.1016/j.apgeochem.2013.07.002.

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- 12. Stewart, I. T. (2009), Changes in snowpack and snowmelt runoff for key mountain regions, *Hydrol Process*, 23(1), 78-94, DOI: 10.1002/hyp.7128.
- 13. Stewart, I. T., D. R. Cayan, and M. D. Dettinger (2005), Changes toward earlier streamflow timing across western North America, *J Climate*, *18*(8), 1136-1155, DOI: 10.1175/Jcli3321.1.
- Todd, A. S., A. H. Manning, P. L. Verplanck, C. Crouch, D. M. McKnight, and R. Dunham (2012), Climate-change-driven deterioration of water quality in a mineralized watershed, *Environmental science & technology*, 46(17), 9324-9332, DOI: 10.1021/es3020056.
- 15. Williams, A. P., et al. (2013), Temperature as a potent driver of regional forest drought stress and tree mortality, *Nat Clim Change*, *3*(3), 292-297, DOI: 10.1038/Nclimate1693.

Journal	JIF 5yr	Count of articles
Nature Biotechnology	46.223	1
Nature	43.769	2
Nature Microbiology	27.755	2
Nature Geoscience	14.35	1
Nature Communications	13.092	2
Isme Journal	11.63	2
Frontiers in Ecology and the Environment	10.841	1
Proceedings of the National Academy of Sciences of the United States of America	10.414	1
Trends in Microbiology	10.239	1
Advances in Colloid and Interface Science	9.446	1
Environmental Science & Technology	6.96	6
Environmental Microbiology	5.965	2
Science of the Total Environment	5.102	1
Hydrology and Earth System Sciences	5.064	1
Environmental Modelling & Software	4.979	1
Geochimica Et Cosmochimica Acta	4.847	1
Scientific Reports	4.847	1
Water Resources Research	4.703	3
Geophysical Research Letters	4.579	1
Frontiers in Microbiology	4.526	1
Biogeochemistry	3.964	1
Journal of Environmental Sciences	3.243	1
Ecohydrology	2.954	1
Computers & Geosciences	2.818	1
Environmental Science-Processes & Impacts	2.706	1
Journal of Contaminant Hydrology	2.559	1
Vadose Zone Journal	2.426	2
PeerJ	2.354	1
Groundwater	2.254	1
Environmental Earth Sciences	1.844	1
Review of Scientific Instruments	1.616	1
Interpretation-A Journal of Subsurface Characterization	0.699	1
Frontiers in Earth Science	n/a	1
Groundwater Assessment, Modeling, and Management	n/a	2
Handbook of Applied Hydrology	n/a	1

#### Appendix III. SFA Products List (publications, awards, invited talks) Publications - published and in press

Handbook of Metal-Microbe Interactions and Bioremediation:	n/a	1			
Principle and applications for toxic metals					
Procedia Earth and Planetary Science n/a					
Grand Total		52			

#### **2017 Publications**

- 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.
- 2. 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.
- 3. Arora, B., J. A. Davis, N. F. Spycher, W. Dong, and H. M. Wainwright (accepted), Comparison of electrostatic and non-electrostatic models for U(VI) sorption on contaminated sediments and the impact on reactive transport simulation, *Groundwater*.
- 4. 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 Geosci, advance online publication*, DOI: 10.1038/ngeo2940.
- 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.
- 6. 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.
- 7. 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.
- 8. 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.
- 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.
- 10. 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.
- 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.
- 12. Varadharajan, C., et al. (2017), Reoxidation of Chromium(III) Products Formed under Different Biogeochemical Regimes, *Environ Sci Technol*, DOI: 10.1021/acs.est.6b06044.
- 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.
- 14. Zaremba-Niedzwiedzka, K., et al. (2017), Asgard archaea illuminate the origin of eukaryotic cellular complexity, *Nature*, *541*(7637), 353-358, DOI: 10.1038/nature21031.

#### **2016** Publications

15. Anantharaman, K., C. T. Brown, D. Burstein, C. J. Castelle, A. J. Probst, B. C. Thomas, K. H. Williams, and J. F. Banfield (2016), Analysis of five complete genome sequences for members of the

class Peribacteria in the recently recognized Peregrinibacteria bacterial phylum, *PeerJ*, 4, e1607, DOI: 10.7717/peerj.1607.

- 16. Anantharaman, K., et al. (2016), Thousands of microbial genomes shed light on interconnected biogeochemical processes in an aquifer system, *Nat Commun*, 7, DOI: 10.1038/ncomms13219.
- Arora, B., D. Dwivedi, S. S. Hubbard, C. I. Steefel, and K. H. Williams (2016), Identifying geochemical hot moments and their controls on a contaminated river floodplain system using wavelet and entropy approaches, *Environmental Modelling & Software*, 85, 27-41, DOI: 10.1016/j.envsoft.2016.08.005.
- Arora, B., et al. (2016), Influence of hydrological, biogeochemical and temperature transients on subsurface carbon fluxes in a flood plain environment, *Biogeochemistry*, 127(2-3), 367-396, DOI: 10.1007/s10533-016-0186-8.
- 19. Babchin, A. J., R. Bentsen, B. Faybishenko, and M. B. Geilikman (2016), On the capillary pressure function in porous media based on relative permeabilities of two immiscible fluids: Application of capillary bundle models and validation using experimental data, *Advances in Colloid and Interface Science*, 233, 176-185, DOI: 10.1016/j.cis.2015.07.001.
- 20. Brown, C. T., M. R. Olm, B. C. Thomas, and J. F. Banfield (2016), Measurement of bacterial replication rates in microbial communities, *Nat Biotech*, *34*(12), 1256-1263, DOI: 10.1038/nbt.3704.
- 21. Brown, T. B., et al. (2016), Using phenocams to monitor our changing Earth: toward a global phenocam network, *Frontiers in Ecology and the Environment*, *14*(2), 84-93, DOI: 10.1002/fee.1222.
- Burstein, D., C. L. Sun, C. T. Brown, I. Sharon, K. Anantharaman, A. J. Probst, B. C. Thomas, and J. F. Banfield (2016), Major bacterial lineages are essentially devoid of CRISPR-Cas viral defence systems, *Nat Commun*, 7, DOI: 10.1038/ncomms10613.
- 23. Chen, J. S., S. S. Hubbard, K. H. Williams, and D. L. Ficklin (2016), Estimating groundwater dynamics at a Colorado River floodplain site using historical hydrological data and climate information, *Water Resour Res*, *52*(3), 1881-1898, DOI: 10.1002/2015wr017777.
- Cismasu, A. C., K. H. Williams, and P. S. Nico (2016), Iron and Carbon Dynamics during Aging and Reductive Transformation of Biogenic Ferrihydrite, *Environ Sci Technol*, 50(1), 25-35, DOI: 10.1021/acs.est.5b03021.
- Danczak, R. E., S. B. Yabusaki, K. H. Williams, Y. Fang, C. Hobson, and M. J. Wilkins (2016), Snowmelt Induced Hydrologic Perturbations Drive Dynamic Microbiological and Geochemical Behaviors across a Shallow Riparian Aquifer, *Frontiers in Earth Science*, 4(57), DOI: 10.3389/feart.2016.00057.
- 26. Dwivedi, D., B. Arora, S. Molins, and C. I. Steefel (2016), Chapter 19: Benchmarking Reactive Transport Codes for Subsurface Environmental Problems, in *Groundwater Assessment, Modeling, and Management*, edited by D. Thangarajan and V. P. Singh, Taylor & Francis Group.
- 27. Dwivedi, D., B. Dafflon, B. Arora, H. M. Wainwright, and S. Finsterle (2016), Chapter 20: Spatial Analysis and Geostatistical Methods, in *Handbook of Applied Hydrology*, edited by V. P. Singh, McGraw-Hill.
- Faybishenko, B., S. Hubbard, E. Brodie, P. Nico, F. Molz, A. Hunt, and Y. Pachepsky (2016), Preface to the Special Issue of Vadose Zone Journal on Soil as Complex Systems, *Vadose Zone Journal*, 15(2), DOI: 10.2136/vzj2016.01.0005.
- 29. Hug, L. A., B. C. Thomas, I. Sharon, C. T. Brown, R. Sharma, R. L. Hettich, M. J. Wilkins, K. H. Williams, A. Singh, and J. F. Banfield (2016), Critical biogeochemical functions in the subsurface are associated with bacteria from new phyla and little studied lineages, *Environ Microbiol*, 18(1), 159-173, DOI: 10.1111/1462-2920.12930.
- 30. Hug, L. A., et al. (2016), A new view of the tree of life, *Nature Microbiology*, *1*(5), DOI: 10.1038/Nmicrobiol.2016.48.
- Janot, N., et al. (2016), Physico-Chemical Heterogeneity of Organic-Rich Sediments in the Rifle Aquifer, CO: Impact on Uranium Biogeochemistry, *Environ Sci Technol*, 50(1), 46-53, DOI: 10.1021/acs.est.5b03208.

- 32. Jewell, T. N. M., U. Karaoz, E. L. Brodie, K. H. Williams, and H. R. Beller (2016), Metatranscriptomic evidence of pervasive and diverse chemolithoautotrophy relevant to C, S, N and Fe cycling in a shallow alluvial aquifer, *Isme Journal*, 10(9), 2106-2117, DOI: 10.1038/ismej.2016.25.
- 33. Kenwell, A., A. Navarre-Sitchler, R. Prugue, J. R. Spear, A. S. Hering, R. M. Maxwell, R. H. Carroll, and K. H. Williams (2016), Using geochemical indicators to distinguish high biogeochemical activity in floodplain soils and sediments, *Sci Total Environ*, 563, 386-395, DOI: 10.1016/j.scitotenv.2016.04.014.
- Long, P. E., K. H. Williams, S. S. Hubbard, and J. F. Banfield (2016), Microbial Metagenomics Reveals Climate-Relevant Subsurface Biogeochemical Processes, *Trends in Microbiology*, 24(8), 600-610, DOI: 10.1016/j.tim.2016.04.006.
- Maxwell, R. M., L. E. Condon, S. J. Kollet, K. Maher, R. Haggerty, and M. M. Forrester (2016), The imprint of climate and geology on the residence times of groundwater, *Geophysical Research Letters*, 43(2), 701-708, DOI: 10.1002/2015GL066916.
- Newcomer, M. E., S. S. Hubbard, J. H. Fleckenstein, U. Maier, C. Schmidt, M. Thullner, C. Ulrich, N. Flipo, and Y. Rubin (2016), Simulating bioclogging effects on dynamic riverbed permeability and infiltration, *Water Resour Res*, 52(4), 2883-2900, DOI: 10.1002/2015wr018351.
- 37. Pribulick, C. E., L. M. Foster, L. A. Bearup, A. K. Navarre-Sitchler, K. H. Williams, R. W. H. Carroll, and R. M. Maxwell (2016), Contrasting the hydrologic response due to land cover and climate change in a mountain headwaters system, *Ecohydrology*, 9(8), 1431-1438, DOI: 10.1002/eco.1779.
- Shiel, A. E., T. M. Johnson, C. C. Lundstrom, P. G. Laubach, P. E. Long, and K. H. Williams (2016), Reactive transport of uranium in a groundwater bioreduction study: Insights from high-temporal resolution U-238/U-235 data, *Geochim Cosmochim Ac*, 187, 218-236, DOI: 10.1016/j.gca.2016.05.020.
- 39. Tinnacher, R. M., D. Dwivedi, J. E. Houseworth, M. T. Reagan, W. T. Stringfellow, C. Varadharajan, and J. T. Birkholzer (2016), Chapter 7: Hydraulic Fracturing from the Groundwater Perspective, in *Groundwater Assessment, Modeling, and Management*, edited by D. Thangarajan and V. P. Singh, Taylor & Francis Group.
- 40. Tokunaga, T. K., et al. (2016), Deep Vadose Zone Respiration Contributions to Carbon Dioxide Fluxes from a Semiarid Floodplain, *Vadose Zone Journal*, *15*(7), DOI: 10.2136/vzj2016.02.0014.
- 41. Tran, A. P., B. Dafflon, and S. S. Hubbard (2016), iMatTOUGH: An open-source Matlab-based graphical user interface for pre- and post-processing of TOUGH2 and iTOUGH2 models, *Computers & Geosciences*, *89*, 132-143, DOI: 10.1016/j.cageo.2016.02.006.
- 42. Tran, A. P., B. Dafflon, S. S. Hubbard, M. B. Kowalsky, P. Long, T. K. Tokunaga, and K. H. Williams (2016), Quantifying shallow subsurface water and heat dynamics using coupled hydrological-thermal-geophysical inversion, *Hydrology and Earth System Sciences*, 20(8), 3477-3491, DOI: 10.5194/hess-20-3477-2016.
- 43. Varaljay, V. A., et al. (2016), Functional metagenomic selection of ribulose 1,5-bisphosphate carboxylase/oxygenase from uncultivated bacteria, *Environ Microbiol*, *18*(4), 1187-1199, DOI: 10.1111/1462-2920.13138.
- 44. Wainwright, H. M., A. F. Orozco, M. Bucker, B. Dafflon, J. Chen, S. S. Hubbard, and K. H. Williams (2016), Hierarchical Bayesian method for mapping biogeochemical hot spots using induced polarization imaging, *Water Resour Res*, *52*(1), 533-551, DOI: 10.1002/2015wr017763.
- 45. Wang, W. X., W. H. Sui, B. Faybishenko, and W. T. Stringfellow (2016), Permeability variations within mining-induced fractured rock mass and its influence on groundwater inrush, *Environ Earth Sci*, 75(4), DOI: 10.1007/s12665-015-5064-5.
- Wrighton, K. C., et al. (2016), RubisCO of a nucleoside pathway known from Archaea is found in diverse uncultivated phyla in bacteria, *Isme Journal*, 10(11), 2702-2714, DOI: 10.1038/ismej.2016.53.

47. Yuan, X., J. A. Davis, and P. S. Nico (2016), Iron-Mediated Oxidation of Methoxyhydroquinone under Dark Conditions: Kinetic and Mechanistic Insights, *Environ Sci Technol*, *50*(4), 1731-1740, DOI: 10.1021/acs.est.5b03939.

#### 2015 Publications (not reported in 2016 proposal)

- 48. Keiluweit, M., P. Nico, M. E. Harmon, J. D. Mao, J. Pett-Ridge, and M. Kleber (2015), Long-term litter decomposition controlled by manganese redox cycling, *Proceedings of the National Academy of Sciences of the United States of America*, *112*(38), E5253-E5260, DOI: 10.1073/pnas.1508945112.
- Ntarlagiannis, D., R. Doherty, R. Costa, K. H. Williams, C. Zhang, and P. Soupios (2015), Introduction to special section: Characterization and monitoring of subsurface contamination, *Interpretation-J Sub*, 3(4), Sabi-Sabii, DOI: 10.1190/Int2015-0917-Spseintro.1.
- Roth, E. J., M. E. Mont-Eton, B. Gilbert, T. C. Lei, and D. C. Mays (2015), Measurement of colloidal phenomena during flow through refractive index matched porous media, *Rev Sci Instrum*, 86(11), DOI: 10.1063/1.4935576.
- 51. Shi, Z. Q., D. Fan, R. L. Johnson, P. G. Tratnyek, J. T. Nurmi, Y. X. Wu, and K. H. Williams (2015), Methods for characterizing the fate and effects of nano zerovalent iron during groundwater remediation, *J Contam Hydrol*, 181, 17-35, DOI: 10.1016/j.jconhyd.2015.03.004.
- Tinnacher, R. M., J. D. Begg, H. Mason, J. Ranville, B. A. Powell, J. C. Wong, A. B. Kersting, and M. Zavarin (2015), Effect of Fulvic Acid Surface Coatings on Plutonium Sorption and Desorption Kinetics on Goethite, *Environ Sci Technol*, 49(5), 2776-2785, DOI: 10.1021/es505120s.

#### Awards

- Banfield, J., Named 2017 Goldschmidt Medalist
- Brodie, E. and Nico, P. LBNL 2016 Director's Award for Service Achievement for National Microbiome Initiative (NMI); developing the science vision for BioEPIC; and for building the case towards CD0 for this \$100M facility.
- Hubbard, S., 2016 Near Surface Hal Mooney Award, Society of Exploration Geophysicists
- Wainwright, H., LBNL 2016 Director's Award for pioneering zonation-based estimation methodologies, with a focus on novel approaches that use geophysical data and their application to DOE challenges in environmental remediation, carbon cycle, and water resources

#### Scientific Leadership (Editorship, Advisory Boards, etc)

- 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
- Brodie, E., CESD Program Domain Lead, Environmental & Biological Systems Science
- Brodie, E., Deputy Division Director, Climate & Ecosystem Science Division (CESD)
- 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 subcomittee
- Dafflon, B., member of writing committee for DOE report on aerial measurements and needs
- Dafflon, B., Member, AGU Hydrogeophysics Technical Committee
- Faybishenko, B., International Atomic Energy Agency (IAEA), Technical Expert and Consultant: Leader of the Technical Group on Decommissioning and Remediation of the Chernobyl Cooling Pond

- Faybishenko, B., Senior Editor, Environmental Sciences, Oxford Research Encyclopedia, Oxford University Press
- Hubbard, S.S., Advisory Board: Interoperable Design of Extreme-Scale Application Software (IDEAS)
- Hubbard, S.S., Director's Council, UC Water (PI Roger Bales)
- Hubbard, S.S., Advisory Board: Radionuclide Waste Disposal: Development of Multi-scale Experimental and Modeling Capabilities, EPSCoR Program, Clemson (PI Brian Powell)
- Hubbard, S.S., ASCEM Sr. Advisor (PI Paul Dixon)
- Hubbard, S.S., Council Member: California Council of Science and Technology (CCST)
- Hubbard, S.S., Civil and Environmental Engineering Advisory Council UCB (Chair R Harley)
- Hubbard, S.S., Cyclotron Road Leadership Council (Director I Gur)
- Hubbard, S.S., Scientific Advisory Board, NSF Arctic Data Center (PI Matt Jones, UCSB)
- Hubbard, S.S., Advisory Board, International Soil Modeling Consortium (ISMC, Harry Veercken, Juelich)
- Hubbard, S.S., Sr. Advisor, ESS-Dive Project (Agarwal, PI)
- Wainwright, H.M., Member, Leadership Team for Berkeley Institute of Resilient Communities
- Williams, K.H., Associate Editor, JGR-Biogeosciences
- Williams, K.H., CESD Program Lead, Environmental Remediation & Water Resources
- 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

#### Invited/Keynote presentations (partial list)

- 1. Arora, B., "Modeling the impact of biogeochemical hotspots and hot moments on carbon fluxes from a flood plain site: Implications for the River Ganges cleanup", IIT Kanpur, Kanpur, IN, January, 2016 (Invited).
- 2. Arora, B., E. L. King, N. F. Spycher, C. I. Steefel, and M. E. Conrad, "Genome-informed reactive transport simulations of CO2 and carbon isotope dynamics in a flood plain aquifer", Goldschmidt Conference, Yokohama, JP, June, 2016 (Invited).
- Beller, H. R., et al., "Omics-enabled discovery of a novel bacterial enzyme enabling first-time biobased toluene production". 12th Annual DOE JGI Genomics of Energy & Environment Meeting, Walnut Creek, CA, March 23, 2017 (Invited).
- Brodie, E. L., "Genome-informed trait based modeling of microbial communities in soil and subsurface systems", Department of Earth System Science, Stanford University, Palo Alto, CA, May, 2016 (Invited).
- 5. Brodie, E. L., "Plenary presentation: Reactive transport modeling in the genomic era", DOE ESS PI Meeting, Potomac, MD, April, 2016 (Invited).
- Dwivedi, D., C. I. Steefel, E. Woodburn, B. Kallemov, D. Moulton, E. Kikinzon, E. Coon, G. Hammond, L. Foster, and R. Maxwell, "Testing Code Interoperability and Productivity on Modeling Integrated Surface Subsurface Water Flow and Biogeochemical Cycling in the Hyporheic Zone IDEAS Use Case 1", DOE ESS PI Meeting, Potomac, MD, April, 2016 (Invited).
- 7. Faybishenko, B., "Groundwater Transport", Origins and Movements of Subsurface Microbes Workshop, University of Southern California, Los Angeles, CA, May, 2016 (Invited).
- Hubbard, S. S., and et al., "Effects of Climate Change on Watershed Dynamics: Insights Gained Using Geophysical Methods", Geotech/Geoengineering Distinguished Graduation Lecture, UC Berkeley, May, 2016
- Hubbard, S. S., et al., "H13L-1582: Predicting Mountainous Watershed Biogeochemical Dynamics, Including Response to Droughts and Early Snowmelt", AGU Fall Meeting, San Francisco, CA, December, 2016
- 10. Hubbard, S.S., France National Polytechnical Institute, Bordeaux, July, 2016

- Hubbard S.S et al., CUAHSI Biennial Colloquium, Finding Your Place in Big Data: Using Observations to Understand Hydrological Processes for Predicting a Changing World, Shepherdstown, WV, July 2016
- 12. Hubbard, S.S, et al, University of Saskatchewan Saskatoon Distinguished Lecturer series, Sept 2016
- 13. Hubbard, S.S. et al. UC Berkeley Civil and Environmental Engineering Seminar March 2017
- 14. Hubbard S.S et al, 27th Annual International Conference on Soil, Water, Energy, & Air, March 20-23, 2017 San Diego, CA Platform presentation
- 15. Hubbard S.S et al. University of Southern California Distinguished Seminar March 2017
- Newcomer, M. E., et al., "B31H-0573: Hydrological and Climate Controls on Hyporheic Contributions to River Net Ecosystem Productivity", AGU Fall Meeting, San Francisco, CA, December, 2016 (Invited).
- 17. Nico, P. S., "Subsurface Reactive Oxygen Species and Implications", DOE ESS PI Meeting, Potomac, MD, April, 2016 (Invited).
- Nico, P. S., "From Aerosols to Oaks: Stories of how transition metals and reactive oxygen species impact our air, land, and water", ESPM Department Seminar, UC Berkeley, Berkeley, CA, April, 2016 (Invited).
- 19. Williams, K.H., "Watershed Function Scientific Focus Area: Hydrobiogeochemistry from the Catchment to Basin Scale", Colorado Water Workshop 2017, Western State Colorado University, Gunnison, CO, June 21, 2017

## Abstracts/presentations to conferences and session convening by SFA members relevant to project (partial list)

- 1. AGU booklet 2016 Full listing | Abbreviated (2 page)
- 2. Anantharaman, K., et al., "Extensive genomic reconstruction provides insights into biogeochemical cycling in a complex terrestrial subsurface environment", JGI User Meeting, 2016.
- Arora, B., D. Dwivedi, C. I. Steefel, N. Spycher, P. M. Fox, and P. S. Nico, "B22B-04: Mineralogical Controls on Carbon Cycling in a Floodplain Environment", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 4. Bearup, L. A., K. W. Williams, and R. W. H. Carroll, "Linking high resolution snow observations, isotope data, and hydrologic modeling to investigate streamflow partitioning in the East River watershed", NASA ASO Workshop, Pasadena, CA, June, 2016.
- 5. Bearup, L. A., R. W. H. Carroll, K. H. Williams, and R. M. Maxwell, "H51N-06: Observing and Modeling Snow Processes Across Spatial and Temporal Scales in Rocky Mountain Headwater Catchments", AGU Fall Meeting, San Francisco, CA, December, 2016.
- Beller, H. R., T. N. M. Jewell, U. Karaoz, M. Bill, R. Chakraborty, E. Brodie, and K. H. Williams, "B14D-08: Strain-resolved Metatranscriptomic Analysis Reveals Unexpectedly Diverse Heterotrophic and Lithoautotrophic Microbial Metabolism in Naturally Reduced Aquifer Sediments", AGU Fall Meeting, San Francisco, CA, December, 2016.
- Bill, M., M. E. Conrad, T. K. Tokunaga, C. Hobson, and K. H. Williams, "B23E-0643: Cycling of greenhouse gases as a function of groundwater level in a floodplain - carbon dioxide, nitrous oxide and methane: Implications for Biogeochemical Change in a Warming World", AGU Fall Meeting, San Francisco, CA, December, 2016.
- Bucksch, A., Y. Wu, T. Scheibe, and N. J. Hess, "B51G: Revealing the Hidden Half: Advances in Imaging and Quantification of Plant Roots and Root-Soil Interactions I Posters", AGU Fall Meeting, San Francisco, CA, December, 2016 (Conveners).
- Bucksch, A., Y. Wu, T. Scheibe, and N. J. Hess, "B54D: Revealing the Hidden Half: Advances in Imaging and Quantification of Plant Roots and Root-Soil Interactions II", AGU Fall Meeting, San Francisco, CA, December, 2016 (Conveners).
- Conrad, M. E., N. J. Bouskill, T. K. Tokunaga, M. Bill, and K. H. Williams, "Nitrate-dependent oxidation of Fe-sulfides in naturally bioreduced zones of floodplain sediments driven by groundwater fluctuations", Goldschmidt Conference, Yokohama, JP, June, 2016.

- 11. Dwivedi, D., C. I. Steefel, B. Arora, and G. Bisht, "How important is the hyporheic zone for large scale biogeochemical cycling?", Goldschmidt Conference, Yokohama, JP, June, 2016.
- 12. Dwivedi, D., et al., "H52D-04: Outsized impacts of hyporheic exchange on coupled carbon and nitrogen cycling in river systems", AGU Fall Meeting, San Francisco, CA, December, 2016.
- Faybishenko, B., T. K. Tokunaga, Y. Kim, and D. Agarwal, "B13E-0668: Uncertainty Propagation in Predictions of Hydraulic Parameters Based on the Pedotransfer Functions", AGU Fall Meeting, San Francisco, CA, December, 2016.
- Foster, L., and R. M. Maxwell, "H51E-1528: Using integrated modeling to study the effect of grid resolution on hydrologic response to climate change in headwaters catchments", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 15. Hubbard, S., Wainwright, H., Tran A., Leger, E., Wu, Y., Dafflon, B., Monitoring, Scaling and Predicting Interactions across Critical Zone Compartments Using Geophysical Data, The 3<sup>rd</sup> AGU-SEG Hydrogeophysics Workshop: Imaging the Critical Zone, Stanford, CA, 2017
- Hsu, H.-T., C. R. Lawrence, M. J. Winnick, J. L. Druhan, K. H. Williams, K. Maher, G. R. Rainaldi, and M. E. McCormick, "B41D-0468: A Molecular Investigation of Soil Organic Carbon Composition, Variability, and Spatial Distribution Across an Alpine Catchment", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 17. Jewell, T. N. M., U. Karaoz, E. L. Brodie, K. H. Williams, and H. R. Beller, "Strain-specific metatranscriptomic evidence of pervasive and diverse chemolithoautotrophy relevant to C, S, N, and Fe cycling in a shallow alluvial aquifer", ASM 116th General Meeting, Boston, MA, June, 2016.
- King, E., E. Brodie, K. Anantharaman, U. Karaoz, N. Bouskill, J. F. Banfield, C. I. Steefel, and S. Molins, "B32A-08: A New Approach to Predict Microbial Community Assembly and Function Using a Stochastic, Genome-Enabled Modeling Framework", AGU Fall Meeting, San Francisco, CA, December, 2016.
- King, E. L., S. Molins, U. Karaoz, K. Anantharaman, N. J. Bouskill, H. R. Beller, J. F. Banfield, C. I. Steefel, and E. L. Brodie, "Development of a stochastic genome-informed trait based model for biogeochemical processes", Computational Methods in Water Resources conference, Toronto, Ontario, June, 2016.
- 20. Lunzer, J., K. H. Williams, H. F. Malenda, and A. Nararne-Sitchler, "ED31B-0883: Analysis of the geochemical gradient created by surface-groundwater interactions within riverbanks of the East River in Crested Butte, Colorado", AGU Fall Meeting, San Francisco, CA, December, 2016.
- Malenda, H.F., Guryan, G., Stauffer, S., Rowland, J., Singha, K. A Meander-scale field investigation of linkages between fluvial geomorphology and patterns of hyporheic exchange. Am. Geophys. Union (12-16 December 2016). Paper No. H33J-1691.
- 22. Malenda, H.F., Williams, K.H., Rowland, J.C., and Singha, K. Real rivers have: A field investigation quantifying river sinuosity's effect on hyporheic exchange: Geol. Soc. of America Abstract Annual Meeting in Denver, Colorado (25-28 September **2016**). Paper No. 157-9.
- 23. Mary, B., Peruzzo, L., Boaga, J., Schmutz, M., Wu, Y., Hubbard, S. and Cassiani, G., "Small scale characterization of vine plant root zone via 3D electrical resistivity tomography and Mise-à-la-Masse method: a case study in a Bordeaux Vineyard," Geophysical Research Abstracts, Vol. 19, EGU2017-Preview, General Assembly, 2017
- 24. Matheus-Carnevali P., Williams, K., Dong, W., Hubbard, S. and Banfield, J., Genome-resolved metagenomic and geochemical analysis of East River riparian zone soils supports the 'systems within systems' approach for watershed analysis, JGI PI meeting, 2017.
- 25. Paul, B. G., et al., "B13J-04: Subsurface metagenomes uncover a vast repertoire of hypervariable proteins encoded by genetic elements in uncultivated organisms and viruses", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 26. Peruzzo, L., M. Schmutz, S. Hubbard, and M. Franceschi, "Evaluation of copper mobility with SIP and geochemical analysis: First results", International Workshop on Induced Polarization (IP2016), Aarhus, Denmark, June, 2016.

- 27. Rainaldi, G. R., M. J. Winnick, C. R. Lawrence, M. E. McCormick, H.-T. Hsu, J. L. Druhan, K. H. Williams, and K. Maher, "B33B-0598: The Role of Alpine Wetlands as Hot Spots of Dissolved Organic Carbon Fluxes in the East River, Colorado", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 28. Siirila-Woodburn, E. R., C. I. Steefel, J. D. Moulton, and D. Dwivedi, "H42C-05: Anthropogenic triggers on the hyporheic zone: quantifying groundwater-surface water interaction and the impact on water quality", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 29. Sutfin, N. A., J. C. Rowland, M. Fratkin, S. J. Stauffer, W. S. Brown, R. W. H. Carroll, K. H. Williams, and G. Perkins, "EP23B-0963: Seasonal and annual shifts in the role of floodplains as sources and sinks of organic carbon", AGU Fall Meeting, San Francisco, CA, December, 2016.
- Tinnacher, R. M., A. Bhattacharyya, P. M. Fox, and P. S. Nico, "B41F-0517: Organic Carbon Release from Groundwater Sediments under Changing Geochemical Conditions", AGU Fall Meeting, San Francisco, CA, December, 2016.
- Varadharajan, C., B. Faybishenko, R. Versteeg, D. Agarwal, S. S. Hubbard, and V. Hendrix, "IN11E-05: Management and assimilation of diverse, distributed watershed datasets", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 32. Wainwright, H. M., and B. Arora, "B32A: Characterizing Spatial and Temporal Variability of Hydrological and Biogeochemical Processes across Scales I", AGU Fall Meeting, San Francisco, CA, December, 2016 (Conveners).
- Wainwright, H. M., and B. Arora, "B33B: Characterizing Spatial and Temporal Variability of Hydrological and Biogeochemical Processes across Scales II Posters", AGU Fall Meeting, San Francisco, CA, December, 2016 (Conveners).
- 34. Wainwright, H. M., C. F. Steefel, K. H. Williams, S. S. Hubbard, B. J. Enquist, H. Steltzer, and S. Trutner, "H11D-06: Mapping Drought Sensitivity of Ecosystem Functioning in Mountainous Watersheds: Spatial Heterogeneity and Geological-Geomorphological Control", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 35. Wainwright, H., et al., "Effective Long-term Monitoring Strategies by Integrating Reactive Transport Models with in situ Geochemical Measurements", Waste Management Conference, Pheonix, AZ, March, 2016.
- 36. Wainwright, H., et al, Multi-type Multiscale Observation Platforms for Quantifying and Scaling Above and Below-ground Interactions, 2nd Asian Conference on Permafrost, ACOP 2017, Sapporo, Japan, July 2-6, 2017
- 37. Wan, J., Tokunaga, T., Dong, W., Williams, K., Hobson, C., Kim, Y., Conrad, M., Bill, M., Long, P. and Hubbard, S., Relative Carbon Fluxes from Soil, Deep Vadose Zone and Groundwater to Atmosphere and River of a Semi-Arid Floorplain in Colorado, GSA Annual Meeting, Denver, CO, September 27, 2016
- 38. Williams, K. H., "H34C-02: The East River, Colorado Community Watershed: Hydrogeochemical Studies Spanning Scales and Disciplines", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 39. Winnick, M. J., R. W. H. Carroll, K. H. Williams, R. M. Maxwell, and K. Maher, "V13B-2845: Concentration-Discharge Relationships, Nested Reaction Fronts, and the Balance of Oxidative and Acid-Base Weathering Fluxes in an Alpine Catchment, East River, Colorado", AGU Fall Meeting, San Francisco, CA, December, 2016.
- 40. Wu, Y., S. S. Hubbard, and B. Dafflon, "Complex resistivity for dynamic imaging of plant root traits and root soil interactions", 4th International workshop on induced polarization, Aarhus, Denmark, June, 2016.
- 41. Yabusaki, S., et al., "Rifle floodplain water table dynamics: biogeochemical cycling and uranium mobility", DOE ESS PI Meeting, Potomac, MD, April, 2016.
- 42. Yuan, X., P. S. Nico, K. H. Williams, X. Huang, and J. A. Davis, "Dark production of hydrogen peroxide in groundwater at Rifle, Colorado", Goldschmidt Conference, Yokohama, JP, June, 2016.

#### **DOE & Community Service and Outreach**

- Brodie, E.L., development team member and narrator for YouTube video "Microbes to Biomes at Berkeley Lab" describing the M2B initiative. http://m2b.lbl.gov/
- Brodie, E.L., interviews with Agricultural publications to present the concepts of beneficial microbiomes to practicing farmers. http://www.agadvance.com/issues/jun-2015/welcome-to-the-microbiome.aspx
- Brodie, E.L., Kavli Foundation Google Hangout discussion on the interface between nanotechnology and microbiome research along with related podcasts. http://www.kavlifoundation.org/science-spotlights/thinking-smaller-how-nanoscience-can-help-us-understand-natures-many-microbiomes
- Brodie, E.L., presented 16 briefings on environmental microbiology various groups and visitors including to USAID, DOE, Monsanto, various VCs, the CA Natural Resource Agency, and Congressman Bruce Westerman.
- Brodie, E.L., presented original curriculum "Life in the Soil" at UC Berkeley Clark Kerr Child Development Center pre-school class. Involves hands-on experiments showing how soil 'breathes' and the life it contains from microbes to springtails, worms and beetles.
- Chakraborty, R., Mentor for TechWomen program
- Hubbard, S.S., Participant and Writer, BERAC Grand Challenge Workshop/Report, 2017
- Hubbard, S.S., Served final term as BERAC member
- Hubbard, S.S. and P. Nico presentation Nature Conservancy Jay Ziegler and team, May 2017
- Hubbard SS and P Nico presentation to CA Department of Water Resources, May 2017
- Hubbard, SS, briefing to Lixin Wu, Director of the Qingdao National Laboratory for Marine Science and Technology, May 2017
- SFA team members (many) participation in DOE SBR Visioning workshop, May 2017
- Steltzer, H. and team have used significant social media to share SFA vegetation research with the greater community. For May/June 2017, Heidi took over the American Geophysical Union Instagram account, sharing photos and stories from the field site with nearly 10,000 followers. An SFA based story on Heidi's science and social media efforts are provided at <a href="https://eesa.lbl.gov/snowmelt-science-mountain-watershed/">https://eesa.lbl.gov/snowmelt-science-mountain-watershed/</a>
- Steltzer, H., ongoing significant social media presence communicating Watershed science to a broader audience follow @heidimountains on twitter and Instagram; @heidisteltzermountains on facebook; and blogs that began last year on the website for the Mountain Research Institute, which will be shifted to @heidimountains on Medium.com.
- Stelzer, H., interviewed for a national radio talk show to share insights on mountain science on May 23, 2017.
- Steltzer, H., shared study design and methodologies through presentations in November 2016 with the Colorado Department of Public Health and the Environment, EPA region 8 and the Niwot Ridge LTER.
- Wainwright, H.M., LBNL POC for National Lab Day on Environmental Management, lead several national labs on the theme "Understanding Earth Systems"
- Wainwright, H.M., Member of DOE CESD-ESS cyberinfrastructure working group
- Williams, K.H., briefing to U.S. Congressman Scott Tipton (R-CO), August 2016
- Williams, K.H., reviewer for LANL LDRD "Critical Watersheds" Project (PI, Richard Middleton)
- Williams, K.H., member of writing committee for DOE workshop on Terrestrial-Aquatic Interface
- Williams, K.H. Executive committee member of DOE CESD-ESS cyberinfrastructure working group

#### Appendix V. Scientific Advisory Board

The Watershed Function SFA formed a new Scientific Advisory Board (SAB) in late 2016. The SAB is requested to provide advice, guidance, connections and constructive feedback to help continuously improve the SFA, as well as to facilitate collaborations that help to extend the SFA impact. In March 2017, the SFA executive committee prepared and delivered a presentation to the members of the SAB to orientate them to our project and provide a first opportunity to receive their comments, questions, and suggestions. Below are short bios for the 11 members of the Watershed Function Scientific Advisory Board.

#### **James Eklund**

Director Colorado Water Conservation Board Department of Natural Resources Denver, CO

As director of the CWCB, Eklund leads the state's water policy and planning efforts and is heading up the development of the Colorado Water Plan. Prior to leading CWCB, Eklund was senior deputy legal counsel to Governor John Hickenlooper, where he focused on key legislative and legal matters, often pertaining to water and natural resources including state water rights, the reorganization of state wildfire responsibilities and groundwater concerns in the South Platte River Basin. While at the State Attorney General's office from 2006 to 2010, Eklund provided legal expertise on many issues central to water policy and planning in Colorado. He represented the Colorado Department of Natural Resources, CWCB and the State Engineer's Office in compact negotiations with other western states, the federal government and Mexico. He provided counsel related to compliance with the Endangered Species Act and water quality laws, and worked in several roles to protect state interests on the Colorado River. Eklund is a fifth-generation Coloradan from the Western Slope.

#### **Alejandro Flores**

Associate Professor Geosciences Department Boise State University

Dr. Alejandro (Lejo) Flores received the BS degree in Civil Engineering from Colorado State University in 2001 and MS degree in Civil Engineering from Colorado State in 2003. In 2009, he received the PhD degree in Hydrology from MIT. His formal training is in watershed modeling, remote sensing and data assimilation. More recently Dr. Flores's research seeks to integrate the role of humans in landscape change, particularly in agriculture and management of public lands, using agent based models. His work also focuses on embedding models of human activity into regional climate models to deduce feedbacks between humans, their actions, and regional hydroclimate systems.

#### **David Gochis**

#### Scientist

#### National Center for Atmospheric Research

Dr. Gochis has conducted field observation and modeling research at the National Center Atmospheric Research (NCAR) since 2002. His academic background is inter-disciplinary between the meteorological and hydrological sciences and civil and agricultural engineering disciplines having earned degrees in both Atmospheric Sciences and Hydrology and Water Resources. Prior to returning to academia, Dr. Gochis worked as a consulting engineer for CH2MHill in Portland, Oregon, conducting channel hydraulics, water resource and irrigation design studies. His current research interests include hydrometeorology, hydroclimatology, and land surface hydrology. His main research foci have been on observation, diagnosis and modeling of precipitation, snowpack and runoff processes in complex terrain with specific emphasis on the inter-mountain west and monsoon systems. Dr. Gochis has led and collaborated in several domestic and international field campaigns. His research develops and employs weather, climate and hydrological

models, to improve understanding and prediction of regional hydrometeorological and hydroclimatological processes. Most recently Dr. Gochis helped lead the implementation of the community WRF-Hydro system as the first version of the NOAA National Water Model.

#### Michael N. Gooseff

Associate Professor Institute of Arctic and Alpine Research Civil, Environmental, & Architectural Engineering University of Colorado

Dr. Gooseff's research group studies the intersection of earth systems and ecosystems, conducting field studies and developing new models to interrogate hydrologic and ecological functions. His group studies the changes in system function in response to changes in boundary conditions and state changes. They have active research programs in the Alaskan Arctic, the McMudro Dry Valleys of Antarctica, and temperate watersheds in the US. The scope of their studies often includes river corridors, aquifers, and glaciers to focus on processes such as nutrient uptake/retention, stream/groundwater interactions, hyporheic exchange, and responses to climate change.

#### **Praveen Kumar**

Lovell Professor of Civil and Environmental Engineering Director, IML-CZO (<u>Critical Zone Observatory for Intensively Managed Landscapes</u>) Department of Civil and Environmental Engineering

#### University of Illinois

Praveen Kumar holds a B.Tech. (Indian Institute of Technology, Bombay, India 1987), M.S. (Iowa State University 1989), and Ph.D. (University of Minnesota 1993), all in civil engineering, and has been on the UIUC faculty since 1995. He is also a Professor in Institute for Sustainability, Energy, and Environment (iSEE), an Affiliate Faculty in the Department of Atmospheric Science and National Center for Supercomputing Applications (NCSA). His research focus is on Hydrocomplexity, which deals with complex hydrologic systems bridging across theory, modeling, and informatics. He presently serves as the Director of the NSF funded Critical Zone Observatory for Intensively Managed Landscapes, which is part of a national and international network. Dr. Kumar is also a co-lead on two large NSF supported SEAD and Brown Dog projects for the development of cyber-infrastructure for structured and unstructured long-tail data, respectively. He has been an Associate of the Center for Advanced Studies, and two-times Fellow of the National Center for Super Computing Applications. He is an AGU Fellow and the recipient of the Xerox Award for Research, and Engineering Council Award for Excellence in Advising. From 2002-2008, he served as a founding Board member for CUAHSI, a consortium of over 110 universities for the advancement of hydrologic science. From 2009-2013, Dr. Kumar served as the Editor-in-Chief of Water Resources Research, the leading journal in hydrology. Prior to that he also served as the Editor of Geophysical Research Letters, a leading journal for inter-disciplinary research. He presently serves as the intellectual leader and Program Advisor for a large effort in India aimed at capacity building through novel approach to research and international collaboration to address the most vexing water problems.

#### **Noah Molotch**

Associate Professor of Geography, University of Colorado at Boulder Director, Center for Water Earth Science & Technology (CWEST) Research Scientist, Jet Propulsion Laboratory, California Institute of Technology Fellow, Institute of Arctic and Alpine Research

Dr. Molotch's research and teaching interests are focused on the processes controlling hydrologic fluxes in semi-arid regions. His research projects utilize ground-based observations, remote sensing, and computational modeling to obtain comprehensive understanding of hydrological processes; in particular the distribution of snowmelt, soil moisture and streamflow. Additional projects aim at developing techniques for scaling hydrological processes and for designing ground-based observation networks

tailored for integration with remote sensing and modeling. Studies relating fluxes of water, carbon, and nitrogen are also a focus of Dr. Molotch's current projects — in particular, the feedbacks between water availability and carbon cycling in montane forests.

#### Scott Saleska

#### Associate Professor Ecology and Evolutionary Biology University of Arizona

Dr. Saleska's research focuses on what might be called "biogeochemical ecology," asking questions about how climate interacts with plant physiology, demography, and ecological processes to influence or control biogeochemical cycling from local to global scales. Just one example of the need for more complete understanding in this area is the lack of species interactions in modern global climate models, even though such interactions can be critically important in controlling ecosystem carbon cycling and hence, feedbacks to climate. Progress has been limited by the difficulty of bridging the gap between local-scale ecological interactions and broader biogeochemical processes. Dr. Saleska uses multidisciplinary approaches that combine classical techniques of field ecology and forestry with advanced technological methods (e.g., the micrometeorological eddy covariance method, isotopic techniques) and modeling to integrate biogeochemical processes to ecosystem scales.

#### Katherine (Katie) Suding

Professor Ecology and Evolutionary Biology Institute of Arctic and Alpine Research University of Colorado Boulder

Dr. Suding is a plant community ecologist working at the interface of ecosystem, landscape and population biology. Dr. Suding's goal is to apply cutting-edge "usable" science to the challenges of restoration, species invasion, and environmental change. Suding's research group works with a range of conservation groups, government agencies and land managers to provide evidence-based solutions that take into account biodiversity, human well-being, and management opportunities. They employ a combination of long-term monitoring, modeling and experimental approaches in settings that range from alpine tundra to oak woodlands to grasslands. Common themes include plant-soil feedbacks, functional traits, species effects on ecosystem processes, and non-linear and threshold dynamics.

#### **Christina Tague**

#### Associate Professor

Bren School of Environmental Science & Management University of California, Santa Barbara

Dr. Tague's research is focused on the interactions between hydrology and ecosystem processes and, specifically, how eco-hydrologic systems are altered by changes in land use and climate. Much of her work involves developing and using spatial simulation models to integrate data from multiple field-based monitoring studies in order to generalize results to larger watersheds. Reflecting that emphasis, Dr. Tague is one of the principal developers of the Regional Hydro-Ecologic Simulation System (RHESSys), an integrated model of spatially distributed carbon, water, and nitrogen cycling. RHESSys is designed to provide science-based information about spatial patterns of ecosystem health and vulnerability in terms of water quantity and quality. Dr. Tague is currently modeling the impacts of climate change on stream-flow patterns in the western United States and examining how urbanization alters drainage patterns and associated biogeochemical cycling in watersheds in Baltimore, Maryland, and Southern California.

#### Philippe Van Cappellen

Canada Excellence Research Chair in Ecohydrology

#### University of Waterloo

Dr. Van Cappellen's research focuses on the biogeochemistry of soils, sediments and aquatic ecosystems, the cycles of water, carbon, nutrients and metals, global change, geobiology, chemical hydrology, water-rock interactions and environmental modeling.

#### Ellen Wohl

Professor Department of Geosciences Colorado State University

Dr. Wohl received a BS in geology from Arizona State University and a PhD in geosciences from the University of Arizona before joining the faculty at Colorado State University in 1989. Dr. Wohl's research interests center on physical process and form in river corridors, as well as interactions among physical processes and biotic and human communities. She has conducted field research on every continent except Antarctica and has authored or co-authored 16 books and nearly 200 peer-reviewed papers. Dr. Wohl is a Fellow of the American Geophysical Union and the Geological Society of America, and has supervised 47 MS theses and 26 PhD dissertations.