An Integrated Measurement and Modeling Approach to Improve Estimates of Water Exports within the East River Watershed

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Abstract:

Evaluation of temporal and spatial changes in water budget components is one of the most critical issues facing water security in mountainous regions. In the East River watershed, efforts within the Water Priority of the Watershed Function SFA have focused on 1) ascertaining sources of uncertainty in water budget quantification, and 2) improving characterization and predictions of water exports in response to disturbances and climatic stressors. To the first point, significant uncertainty is attributed to evapotranspiration (ET) rates. To this end, our efforts have focused on (a) reconciliation of various ET methods used at the East River to identify critical sources of uncertainties, and (b) development of ET benchmarking platforms and datasets to reduce uncertainties. Our synthesis efforts indicate that ET estimates do show some variability across applied methods (e.g., flux tent, water mass-balance, and sap-flow); however, there is consensus regarding transitions between water and energy limited systems across locations and years. Our model and data analyses further indicate that lysimeter-based SMARTSoils testbeds are important

benchmarks to improve consensus across these methods, especially in analyzing the differences in evaporation and transpiration. In addition, a 34-year long analysis on potential ET and aridity index using climatic variables shows temporal shifts in behavior that are distinct but not insignificant across 17 meteorological stations spread across the East River watershed domain (Faybishenko et al., in review). Taken together, these analyses provide key information for identifying critical locations, measurements and modeling approaches for scaling high resolution, local scale ET measurements to the entire watershed with reduced uncertainty.

To the second point, efforts were carried out in the past year to quantify variations in partitions and drivers for streamflow using hydrological modeling and stable isotope approaches. Stable water isotope observations of snow water indicate elevation is a dominant control on the temporal variability of snowmelt input to the subsurface and that streamflow is in fact dominated by snowmelt water (>90 %) throughout the year. These analyses combined with five years of groundwater observations from multiple deep wells are providing evidence that the upper subalpine region is a preferential recharge zone in mountain systems (Carroll et al., in revision). In order to better assess the variability in streamflow generation and identify recharge zones under disturbance, future efforts in the Water Priority are geared towards distributed sampling through isotopes, Snow/Soil Distributed Temperature Profiling, and integrated modeling within and across functional zones.

Carroll, R.W.H., Deems, J., Maxwell, R., Sprenger, M., Brown, W., Newman, A., Beutler, C., Bill, M., Hubbard, S., Williams, K.H. Variability in observed stable water isotopes in snowpack across a mountainous watershed in Colorado, *in revision*, Hydrological Processes.

Faybishenko, B., B.Arora, D.Dwivedi, E. Brodie. Statistical Framework to Assess the Temporal and Spatial Climate Changes: East River Mountainous Watershed case study, *in review*.

How Do Geology and Biology Determine Watershed Nitrogen Export? A Paired Catchment Study

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Abstract:

Nitrogen is a limiting element within mountainous ecosystems. Coarse soils, sparse vegetation, and strong hydrological events, such as snowmelt and monsoonal precipitation, can flush nitrogen prior to assimilation and retention in plant and microbial biomass. However, the role that discrete landscape properties play in determining the retention and release of nitrogen at the watershed scale is poorly understood. Our study focuses on two catchments within the East River watershed in the Upper Colorado River Basin: At 56 km^2, Coal Creek exhibits an east-west orientation, with north- and south-facing hillslope aspects, ~70% land cover by conifer tree species, and bedrock dominated by Upper Cretaceous and Eocene sand- and silt-stones and igneous rock types. The 86 km^2 main stem East River is oriented in a northwest-southeast direction, has 26% coverage by conifer species, and is largely underlain by Cretaceous Mancos shale bedrock, which is entirely absent in Coal Creek. Runoff characteristics for both catchments are similar in terms of the timing of peak discharge in early June and the transition to baseflow in late September-early October, where groundwater represents a significant fraction of streamflow.

These distinguishing characteristics manifest themselves in terms of the concentration magnitude and isotopically inferred source of nitrogen exported from each catchment. For example, the nitrate exported from Coal Creek is sourced primarily from new, atmospherically deposited nitrate, which makes up ~54 % of riverine nitrate. By contrast, nitrate is retained longer in the East River

watershed, where it is cycled multiple times, and when exported, is primarily (~64 %) derived from terrestrial sources. Taken collectively, our multi-year results provide a unique insight into the primary controls on the provenance of nitrogen loading and its riverine export when considered over scales that functionally aggregate to a collective, integrated watershed response.

Finally, using a coarse-resolution model representing the interacting nitrogen and water cycles, we extend our observations to further address how the nitrogen cycle, and, by extension, the availability of nitrogen to plants and microbes, is impacted by climate extremes. Specifically, we perturb the different catchments feeding into the East River watershed by increasing annual temperature and lengthening the summer dry period. These perturbations show a strong impact on nitrogen export, with higher inorganic nitrogen exported under warming conditions. We further demonstrate the important role vegetation plays in the ecosystem retention of nitrogen, and emphasizes the need to improve our understanding of when plants acquire different organic and inorganic nitrogen compounds within mountainous ecosystems.

Fossil Carbon Release and Exports from Subsurface Sedimentary Bedrock Weathering in Mountainous Watersheds

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Abstract:

Chemical weathering of silicate rocks can be a sink for atmospheric CO_2, while weathering of sedimentary rocks can be a source of CO_2 emission. Because sedimentary rocks cover about 2/3 of the Earth's land surface and contain the Earth's largest C inventory as fossil organic carbon (OC_{petro}) and inorganic carbonate (IC_{petro}), it is important to understand contributions of rock weathering to the terrestrial C cycle. Predictive models on C transfer between rocks and atmosphere are based on the estimated rates of tectonic uplift, weathering, and erosion of exhumated rocks on the Earth's surface over geological time scales. Recent critical zone research has advanced towards greater recognition of *sub*surface rock weathering. However, quantifying subsurface weathering rates is limited by knowledge of where the most important weathering reactions take place and depth-dependent water fluxes. This research integrates a range of measurements to develop understanding of modern-day rock weathering impacts on C cycling.

This study was conducted in the East River watershed located in the Upper Colorado River Basin where recharge occurs primarily during snowmelt. Along a lower montane hillslope underlain by Mancos Shale, we drilled several deep boreholes and instrumented them with numerous samplers and sensors. We collected 5 years of time- and depth-resolved hydrological and biogeochemical data, including solid, porewater, and pore-gas chemistry, as well as ^{14}C signatures in solid C, DIC, DOC and CO_2. We found that (1) modern-day sedimentary rock weathering releases DIC_{petro} and DOC_{petro} from a narrow region below the soil, which we define as the weathering zone; the annual water table oscillation determines this zone's thickness and the deepest extent of the water table determines the weathering front. This finding combined with well-constrained subsurface flow

rates allowed quantification of weathering rates. Because vast areas of the Earth's surface are underlain by sedimentary rocks, this new insight on the weathering zone's role in the carbon cycle is important. (2) The dissolved carbon pool in the subsurface consists primarily of DIC_{petro} (~ 85%), which exports through groundwater for eventual CO_2 emission from surface waters. (3) The measurements-based annual release rates from shale bedrock weathering are 85 and 15 kg/ha of IC_{petro} and OC_{petro}, respectively. Our estimated global scale rate of C_{petro} release from subsurface shale bedrock weathering to the environment is about 0.32 Pg per year.

Coupled River Corridor Processes across Scale

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Abstract:

The river corridor processes component of the Watershed Science SFA seeks to examine how the complex coupling of physical, chemical, and biological processes along the river corridor of the East River in Colorado control the local carbon, metal, and nutrient dynamics. At the largest scale the team has shown the heterogeneity of behavior along different reaches of the river, with reaches of similar length showing very different changes (increases/decreases) in the fluxes of specific species, e.g. nitrate, sulfate, DIC, and dissolved cations. The drivers of this difference in behavior are being analyzed in terms of the watershed functional zonation work and in terms of key river corridors features such as floodplain wetland complexes and the confluence of significant tributaries. Further, the observed floodplain dynamics couple with hydrologic perturbations to show how the size of the snowmelt hydrologic pulse impacts the chemical contributions of the floodplain to the river. Reactive transport modeling at the meander to reach scale confirms how river morphology and connectivity to hyporheic exchange exert strong influences on the degree of biogeochemical processing and identifies particular potential locations of concentrated activity. Further, a numerical exploration of river sinuosity as represented by meander amplitude is explored to further understand this impact and present a possibility for scaling motifs. At the smallest scale, the transformation of sulfur species from their origin as a by-product of rock

weathering to their interactions with river stage perturbations is tracked in order to move toward a system scale understanding of key biogeochemical cycles. Similarly, a detailed exploration of microbiological conditions along the river corridor reveal evidence of hyporheic organisms with a capacity for methane oxidation and nitrogen fixation. This insight highlights the complexity of the fundamental process that create the emergent behavior observable at the river corridor scale.

Machine Learning-Based Multi-Scale Multi-Compartment Watershed Characterization across Scales

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Abstract:

Predictive understanding of watershed functions – such as ecosystem dynamics, water fluxes, nutrient cycling and export – is often hindered by the heterogeneous and multiscale fabric of watersheds. In the Watershed Function SFA, we are developing novel watershed-characterization methodologies to quantify complex watershed systems across scales, while taking advantage of recent advances in airborne remote sensing technologies. Machine learning (ML) plays a significant role in identifying and quantifying the relationships between spatially extensive remote sensing data and sparse measurements, like geophysical or in-situ sampling. ML quantifies the co-variability between above/belowground properties and aids in reducing the multi-dimensional parameter space into a set of *watershed zones* to tractably capture these co-varied properties.

In this presentation, we present several key recent developments and findings:

- The effective integration of multiscale geophysical data (borehole, surface, airborne) through ML has enabled the quantification of correlations between topographic/vegetation metrics (obtained from remote sensing data) and bedrock properties, to estimate bedrock properties across the watershed. In particular, this approach also enabled us to map hydrogeologically important features, such as permeable fracture zones.
- A hybrid model that combines a process-based model and empirical relationships was developed to estimate the spatial heterogeneity of soil thickness at fine spatial resolution across

a hillslope, by combining a process-based soil erosion/diffusion model and empirical relationships between topographic metrics and soil thickness.

- A ML-enhanced probabilistic framework was developed to quantify both the parameter and model uncertainty of geological structures based on geophysical data. This framework was applied to identify a new fault, which is a fast groundwater flow path, and which was later confirmed through drilling and core recovery.

- Watershed zonation was identified and mapped through hillslope clustering of airborne remote sensing data (LiDAR, hyperspectral, and electromagnetic surveys). Hillslopes were identified as an appropriate unit for capturing the key bedrock-through-canopy properties dictated by aspects, elevation and geology. Using independently collected data, we show that the identified zones provide information about zone-based watershed functions, including foresummer drought sensitivity and river nitrogen exports.

Through explicitly bridging information derived from “on the ground" observations made at the East River Watershed and remote sensing data, we quantify fundamental scientific linkages among interacting processes in the watershed.

Miltenberger A, Uhlemann S, Mukerji T, et al (2021) Probabilistic Evaluation of Geoscientific Hypotheses With Geophysical Data: Application to Electrical Resistivity Imaging of a Fractured Bedrock Zone. J Geophys Res Solid Earth 126:1–20. https://doi.org/10.1029/2021JB021767

Uhlemann S, Dafflon B, Wainwright HM, et al (2022) Surface parameters and bedrock properties co-vary across a mountainous watershed: Insights from Machine Learning and Geophysics. Science Advances (accepted).

Wainwright HM, Uhlemann S, Franklin M, et al (2022) Watershed zonation through hillslope clustering for tractably quantifying above- and below-ground watershed heterogeneity and functions. Hydrol. Earth Syst. Sci., 26, 429–444. https://doi.org/10.5194/hess-26-429-2022

Yan Q, Wainwright H, Dafflon B, et al (2021) A hybrid data–model approach to map soil thickness in mountain hillslopes. Earth Surf Dyn 9:1347–1361. https://doi.org/10.5194/esurf-9-1347-2021

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

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Abstract:

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

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

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

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

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

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

Xu, S., Molins, S., Ozgen-Xian, I., Dwivedi, D., Svyatsky, D., Moulton, J.D., Steefel, C.I., Understanding the hydrogeochemical response of a mountainous watershed using integrated surface-subsurface flow and reactive transport modeling, *in review* Water Resources Research.

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

Remote Sensing to Scale Plant, Soil and Microbial Traits and to Infer Watershed Temporal Responses to Disturbance such as Forest Decline

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Abstract:

Ecological interactions between plants, microbes and geologic substrates are key to the retention of loss of elements across watersheds. Spatial, temporal, and phylogenetic scales affect interpretation of these interactions. An open question is how to best assess ecological interactions occurring across these scales, and to determine when and where do processes occurring at fine spatial scales affect aggregate watershed function? We are developing strategies to scale plant and microbial traits from point-scale measurements to watershed scales using remote sensing of plant traits and landscape features. By classifying and mapping functionally distinct soil, plant and landscape units our goal is to identify generalizable patterns in plant and microbial traits at the watershed-scale. In this presentation, we will present the following findings:

Characterizing Representative Soil Biogeochemical Units:

More than 400 soils were collected in 2018 across elevations over four catchments which varied in hydrologic, geologic, and vegetation properties. We classified soils into 5 functional categories based on similarity in microbial biogeochemical properties.

Scaling Soil Biogeochemical Properties and Microbial Traits at the Watershed Scale:

We developed machine learning- (ML) approaches that use airborne hyperspectral imaging and LiDAR data to estimate plant functional type and species cover, plant leaf traits such as leaf nitrogen and carbon, and leaf mass per area at both fine spatial scale and at watershed scales.

Remotely-sensed predictions of plant traits were then used to quantify the co-variability between soil microbiomes, soil properties and landscape features. ML approaches have identified predictive plant leaf traits (e.g. leaf water content) and landscape properties (e.g. topographic wetness) that were used to scale soil microbial traits at watershed scale. Using this approach, we identified that soil microbial biomass and nitrogen (N) accumulation follow landscape features related to water availability.

Synthesizing Data and Scaling Frameworks to Infer Temporal Watershed Dynamics:

We have also identified watershed areas of forest decline and biomass loss by analyzing time-series satellite imagery. Strong relationships were found with topographic properties and total potential solar radiation. Such ecosystem relationships and dynamics have implications for watershed N export, and may help explain significant variability in river N exports over the past several decades.

Abundant multi-omic data collected at East River is being used to build an interoperable and dynamic resource to directly parameterize HPC reactive transport models using genome-informed microbial traits. A goal is to improve predictions of the scale at which nitrogen retention and loss is regulated in a watershed.

Shale Weathering in a Mountainous Watershed: Impact of Water Table Fluctuations and Implications for Nitrogen Cycling

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Abstract:

Shale formations represent critical contributors to global nitrogen and carbon cycles due to their widespread occurrence and high content of organic matter and carbonate minerals. In particular, shale bedrock weathering strongly influences the export of solutes and nutrients to rivers, leading to significant release of greenhouse gasses to the atmosphere. Understanding the complex interplay between hydrochemical, biogeochemical, and physical processes that control the transformation of shale bedrock represents a major scientific challenge for the interpretation of seasonal and longer-term cycling of nutrients.

In this study, we develop a modeling approach to quantitatively interpret long-term alteration of shale bedrock and analyze the coupling between shale weathering, seasonal water fluctuation, and the cycles of carbon and nitrogen along a well-instrumented hillslope-to-floodplain transect located in the East River Watershed. The model simulates the exchange of gasses between the atmosphere and the subsurface, the infiltration of meteoric water, a series of microbially-mediated reactions, including the cycling of nitrogen, as well as the transformation of mineral assemblages induced by dissolution/precipitation reactions.

The model results show that the ingress of oxygen drives the dissolution of sulfide minerals and a variety of microbially-mediated reactions. The degradation of organic matter enhances the dissolution of carbonate minerals and leads to significant emission of CO_2 into the atmosphere. In particular, the model indicates that modern organic matter is the primary source of nitrogen due to its relatively high reactivity although fossil shale-associated organic matter and atmospheric N deposition represent important secondary sources. While a large part of the nitrogen denitrifies in the unsaturated zone, dissimilatory nitrate reduction to ammonium represents an important nitrogen retention pathway in the saturated-anoxic zone. The degree of water saturation exerts a

strong control on the gas fluxes, and thus ultimately determines the weathering rates. In particular, the model shows that while the thickness of the weathered front is determined by the greatest depth of the water table, strong water table fluctuations occurring between dry and snow-melt periods result in rapid seasonal shifts in microbially-mediated reactions, mineral dissolution, and nutrients concentrations. On a longer time scale, these water table fluctuations can result in significant changes in the growth and activity of plant types. During low snow years, modeling results highlight the importance of deeper water, and potentially shale-derived nitrogen resources, in preferentially sustaining deep-rooted shrubs over shallow-rooted forbs at mid-slope locations. Finally, efforts are underway to understand how hillslope topography and floodplain retention may interact to impact hydrogeochemical exports to rivers under different snow years.

A Showcase of Integrated Atmosphere-to-Bedrock Science Activities in the East River Watershed to Advance Mountainous Hydrology

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Abstract:

The East River watershed of the Upper Colorado River is now one of the most heavily-instrumented headwater basins in the world through cross-scale investments in scientific activities using measurements, modeling, and analysis of processes that dominate mountainous hydrology from the atmosphere through the bedrock. Established subsurface through canopy observations and models of water, metals, and nutrients via support from the U.S. Department of Energy's Watershed Function Scientific Focus Area project (WF-SFA) are being contextualized with atmospheric measurements obtained from the new Surface Atmosphere Integrated Field Laboratory (SAIL) campaign and partner campaigns including NOAA's Study of Precipitation, the Lower Atmosphere, and Surface for Hydrometeorology (SPLASH). With preliminary data from SAIL and SPLASH and accelerating activities connecting those data to WF-SFA activities, we present a number of examples highlighting the nature of the interdisciplinary research work, in its current working state, that is advancing the science of mountainous hydrology. These include: (1) validating precipitation radar measurements, (2) using these measurements to explore surface

and subsurface water partitioning, (3) improving the mechanistic understanding of connections between atmospheric, surface, and subsurface processes with observationally-constrained integrated process models, (4) constraining snowpack and blowing-snow sublimation using in situ measurements, wind and precipitation measurements, and LiDAR-based snowpack surveys, and (5) exploring how radiation and atmospheric aerosol processes impact nutrient delivery via airborne deposition that, in turn, impact surface and below ground hydro-biogeochemical processes. These advances are critical for strengthening the predictive understanding of water and energy budgets, as well as fluxes of nutrients and metals in the Anthropocene. These examples represent only a subset of those enabled through creation of the Nation's first atmosphere-to-bedrock field observatory. This presentation is intended to spark discussion as to additional interdisciplinary research needed to establish the minimum but sufficient observational datasets required for developing a predictive understanding of watershed system functionality in the Upper Colorado River Basin and other snow-dominated mountainous systems worldwide.

Toward Integrated BioEPIC, Data Management and Assimilation Capabilities Supporting Watershed Research

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Project: Berkeley Lab Watershed Function SFA

Project Website: watershed.lbl.gov

Abstract:

The extreme complexity of natural ecosystems poses significant challenges in the quantitative understanding of critical processes driving system functioning and predictability. Field-scale studies of coupled processes are hindered by our limited capabilities to characterize, monitor, manipulate, and model systems to derive scalable causal functions beyond a local context. We present emerging capabilities for sensing, experimentation, data management and assimilation into models driven by scientific needs to tackle these challenges.

The BioEPIC (Biological and Environmental Program Integration Center) capability developments in support of ecosystem science are centered on challenges and needs driven by community input. Coupled plant-soil-microbial processes represent a key theme, while new sensing capabilities, and manipulative platforms that represent field-scale, yet manageable complexity, are needed. The SMART (Sensors at Mesoscale with Autonomous Remote Telemetry) Soils testbed and EcoSENSE program are developing capabilities to quantify complex causal interactions across plant-soil-microbial-atmosphere interfaces with novel sensing technologies that are transferable from lab to field. Integrating >70 continuous data streams from existing and novel EcoSENSE technologies, the SMARTSoils testbed demonstrated the power of joint utilization of multi-scale and multi-physics datasets in elucidating underlying mechanisms driving ecosystem dynamics. The testbed is used to validate and improve models to quantify evapotranspiration (ET), a major source of uncertainty in the water budget, for the Watershed Function Science Focus Area (WFSFA). With the first prototype completed and fully functioning,

the design and construction of SMARTSoils 2.0 aims to be modularized and standardized to allow easier community adoption.

The WFSFA data management and assimilation framework provides infrastructure to establish field-to-lab connectivity, perform automated data quality checks, and enable data integration. An ongoing effort in partnership with the DOE's ESNet user facility involves establishing telemetric connectivity between Berkeley Lab and the East River watershed observatory via advanced wireless communication (5G and satellite) networks. In parallel, a variety of ML and statistical algorithms are being explored for data screening from field and lab in near real-time. An open source brokering service tool BASIN-3D enables integration of diverse field, lab and external datasets on-demand from distributed data sources into a common format based on the Open Geospatial Consortium's Observations and Measurements.

Together these technologies will enable a rapid, interactive feedback loop between the SMARTSoils platform, the East River watershed observatory, and associated models and data systems. These capabilities are needed to complete the cycle of field-informed experiment execution, lab-informed model parameterization, and optimal model-driven measurement adaptation in the field.