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Investigating Soil Organic Matter Composition and Degradation State Across Hillslope Positions in the Arctic Foothills of Alaska

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BER Program: ESS
Project: Argonne National Laboratory Soil Carbon Response to Environmental Change SFA
Project Website: https://ess.science.energy.gov/anl-sfa/ and http://tessfa.evs.anl.gov/

Project Abstract: In the permafrost region, the soil organic carbon (SOC) stocks of hilly terrains are highly uncertain. In particular, frozen hill-toe soil deposits are one of the highest uncertainties at the circumpolar scale. The vulnerability of SOC stocks to warming depends on ice contents and the amount and composition of soil organic matter (SOM) occurring at different depths across the landscape. In addition to erosion and other processes, hillslopes in the Arctic are impacted by permafrost-affected solifluction and other lateral mass movements, cryoturbation, and patterned-ground formation. These processes might differently affect the accumulation, distribution, and decomposition of SOM across hillslope toposequences. We investigated the composition and degradation state of SOM at different landscape positions across two toposequences formed on differing land surface ages in the Arctic Foothills of Alaska. The soil profiles of seven hillslope positions (summit, shoulder, upper and lower backslope, upper and lower footslope, and basin) were sampled by soil layers to depths of 1-3 m. We determined SOC stocks and water/ice contents at comparable hillslope positions for each toposequence. We also evaluated profile variations in SOM composition (organic functional groups and minerals) and indicators of SOM degradation state by analyzing the mid-infrared spectra of the soil. Both hillslopes contained large SOC stocks to 1-m depth across the toposequence. Volumetric ice content was high at all hillslope positions with pore ice and ice lenses forming a range of soil cryostructures. Ice-wedges were observed at summit, shoulder, lower footslope, and basin positions. A principal component analysis indicated similar SOM composition occurred across all slope positions with the exception of the basin areas, where greater accumulation of non-polar methyl group compounds dominated over other organic functional groups. Indicators of SOM degradation state, such as high ratios of carboxylates to polysaccharides, were negatively correlated with SOC content suggesting that SOM associated with mineral soil layers were more degraded than organic or mixed organic/mineral layers. Next steps will focus on understanding how SOM degradation state varies with the depth distribution of different soil layers across each toposequence — with the aim of generating spatially explicit local and regional estimates of SOM degradation state and potential decomposability for hillslope-dominated arctic landscapes.

Improving Long-Term Modeling of Soil Carbon and Permafrost Response to Wildfire through Observational Evidence in the Southernmost Permafrost Region of Alaska

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Project Abstract: The permafrost-affected soils and ecosystems of the Copper River Basin (CRB) represent the southernmost area of extensive, discontinuous permafrost in Alaska. These soils are considered ecosystem-protected because prevailing ecological conditions, rather than climate alone, are the major influence on permafrost stability. In subarctic and boreal regions, soil carbon and permafrost depth are strongly dependent on the thickness of the surface organic layer, which stores large amounts of carbon at a landscape scale and acts as an insulator to protect permafrost from degradation. Nevertheless, the surface organic layer is extremely sensitive to disturbances such as wildfire. Depending on severity, wildfires can remove or severely reduce the thickness of the organic layer, reduce insulation, and lead to soil carbon loss and permafrost degradation. Many observational and modeling efforts have examined fire-induced changes in organic layer thickness, soil carbon, and permafrost in Interior Alaska over decadal scales. However, the soils, permafrost, and landscapes of the CRB are dominated by clayey, fine-textured soils on flatter terrain with longer fire-return intervals compared to Interior Alaska. Preliminary work has shown that the fire responses of permafrost-affected soils and their carbon stocks in the CRB differ in critical ways from those observed for the generally silty textured, better drained soils of Interior Alaska. Unlike many sites in other permafrost-affected landscapes where soils can become drier following permafrost degradation due to increased drainage, our work has shown that soils in the CRB are more likely to become wetter post-fire. The restrictive permeability of CRB soils, fire-induced loss of transpiration, and low gradient landscapes combine to profoundly influence the long-term trajectory of CRB soils and ecosystems. These factors may lead to dramatically different outcomes with respect to soil carbon balance compared to Interior Alaska, with potentially increased rates of post-fire carbon accumulation due to wetter conditions. Yet, because of relatively warm ambient and permafrost temperatures in the CRB, it is unlikely that permafrost aggradation occurs post-fire by upward freezing from the permafrost table. Rather, the formation of new near-surface permafrost following the recovery of the organic layer may occur simultaneously with the development of taliks. These interacting factors could make CRB soil carbon stocks and permafrost either more or less susceptible to disturbances caused by wildfires and rising annual temperatures.

Quantifying Variations in Soil C:N Relationships for the Permafrost Region

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Project Abstract: Recent worldwide efforts have improved estimates of soil organic carbon (SOC) stocks and their spatial and vertical distributions for the permafrost region. However, predicting the fate of these SOC stocks in response to changing climatic conditions and projecting their impact on carbon-climate feedbacks require better information on additional soil properties. For example, understanding the nitrogen (N) reserves currently held by permafrost-region soils, their relationships with SOC stocks, and their susceptibility to release under changing climatic conditions will be important for efforts to model future ecosystem and regional responses and feedbacks. Soil C:N ratio can be an indicator of decomposability as it can influence microbial decomposition processes—with related effects on N availability, nitrous oxide emissions, and vegetative responses to climatic and hydrologic changes. Yet, efforts to map the patterns of soil N stocks and C:N relationships for the permafrost region currently lag behind those for SOC stocks. The first study to estimate the distribution of soil N stocks across the northern circumpolar region (Palmtag et al., https://doi.org/10.5194/essd-2022-8, in review) used a thematic mapping approach based on land cover classes spatially available at 300-m resolution to upscale a newly available observational dataset. As an important soil forming factor, land cover affects the form and composition (including C:N) of recent organic inputs to soil and also generally reflects the integrated effects of climate and edaphic factors—making it a useful predictor for upscaling studies. In the permafrost region, however, unique cryo-pedogenic processes (such as cryoturbation) and the preservation of poorly degraded soil organic matter at depth suggests the need to investigate soil C:N relationships in the context of other soil forming factors at higher spatial resolutions. However, mapping and interpretation of soil property ratios (including C:N) is challenging, with no set standard, particularly for the heterogeneous profiles of permafrost-affected soils. The drawback to direct mapping of soil C:N is the assumption that similar environmental factors influence the spatial and vertical variability of both SOC and N, which might not be true. Another approach would be to map SOC and N stocks independently, to capture how different environmental factors affect each soil property, and then determine soil C:N distributions from the two digital soil mapping products. In this study, we compare these two approaches at high spatial resolution in Alaska to evaluate which can best capture and explain spatial and vertical variations in soil C:N relationships.

The Argonne National Laboratory Subsurface Biogeochemical Research Program SFA: Wetland Hydrobiogeochemistry

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Project: Argonne Wetland Hydrobiogeochemistry SFA

Project Website: https://doesbr.org/documents/ANL_SFA_flyer.pdf
https://www.anl.gov/bio/project/subsurface-biogeochemical-research

Project Abstract: Within wetlands, movement of water and biogeochemically catalyzed transformations of its constituents determine the mobility of nutrients and contaminants, emission of greenhouse gasses into the atmosphere, carbon (C) cycling, and the quality of water itself. The long-term objective of the Argonne *Wetland Hydrobiogeochemistry* Scientific Focus Area (SFA) is the *development of a mechanistic understanding and ability to model the coupled hydrological, geochemical, and biological processes controlling water quality in wetlands and the implications of these processes for watersheds commonly found in humid regions of the United States.* The Argonne *Wetland Hydrobiogeochemistry* SFA focuses research on a riparian wetland within Tims Branch at the Savannah River Site. Tims Branch contains riparian wetlands representative of those commonly found in humid regions of the Southeast that have C-rich soils and high Fe content. However, it is unique in that parts of the watershed received large amounts of contaminant metals and uranium as a result of previous industrial-scale manufacturing of nuclear fuel and target assemblies. Understanding the function of wetlands in relation to hydrologic exchange, including the concentration of nutrients and contaminants within the soluble and particulate components of groundwater and surface waters addresses the goal of the ESS Program to *advance a robust, predictive understanding of watershed function*.

Biogeochemical Dynamics of Fe and U in Fe Flocs in Tims Branch, Savannah River Site under Oxic/Anoxic Cycling

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Project: Argonne Wetland Hydrobiogeochemistry SFA

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Project Abstract: The Argonne *Wetland Hydrobiogeochemistry* SFA studies are centered on a riparian wetland field site within Tims Branch at the Savannah River Site and are focused on hydrologically driven biogeochemical processes within three critical zones: *sediment, rhizosphere,* and *stream*. The dynamic nature of the processes occurring within the *stream* zone is illustrated by the formation of flocs, which are multicomponent assemblages of microbes, minerals, and non-living organic matter that are often found in freshwater ecosystems, including wetlands. Abundant orange and reddish-brown flocs have been repeatedly observed along gaining sections of Tims Branch, where anoxic groundwater containing Fe(II) contacts oxygenated stream water. Analysis of these flocs by ICP-OES and XAFS spectroscopy revealed that the flocs contain high levels of Fe (8–17 wt%)—primarily in the form of ferrihydrite and lesser amounts of lepidocrocite and Fe-organic complexes as determined by Fe K-edge EXAFS spectroscopy—P (2–4 wt%) and S (1–3%). The flocs also contain 155–600 ppm U in the form of a U(VI) oxyhydroxide phase, as indicated by U L_{III}-edge EXAFS analysis. Flocs can undergo microbially mediated cycling of redox active elements such as Fe and U. Laboratory microcosm studies show that the transition from oxic to anoxic conditions leads to the reduction of Fe(III) to Fe(II) and U(VI) to non-uraninite U(IV); following a return to oxic conditions, Fe(II) and U(IV) oxidize back to Fe(III) and U(VI). Given that Fe flocs are frequently observed in a broad range of wetland environments, our studies of Fe floc biogeochemistry in Tims Branch and its potential impact on U speciation and transport expand our understanding of their role in the speciation and cycling of trace elements in wetlands, which in turn can lead to more robust modeling of trace element behavior in aquatic and terrestrial environments.

Watershed-Scale Hydrobiogeochemical Properties that Cause Contaminant Hot Spots

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Project: Argonne Wetland Hydrobiogeochemistry Science Focus Area (SFA)

Project Website: https://ess.science.energy.gov/anl-wetland-sfa/

Project Abstract: Argonne's Wetland Hydrobiogeochemistry SFA is a multi-scale study of the hydrobiogeochemical processes governing water quality at a uranium (U) contaminated wetland located on the Savannah River Site, Aiken, SC. The objective of this study was to determine hydrological, soil, and topographical properties that influence U concentration distribution along an 8 km reach. The general approach was to create U concentration maps, collect and characterize soil cores for U properties, and then use flow models to test various hypotheses to explain the presence of multi-hectare-sized hot spots of U. Using walk-over gamma mapping techniques, the area previously surveyed was expanded another 30% to ~40 hectares. Based on 400,000 gamma spectra and 10 soil cores, it was determined that 94% of the originally released 43,500 kg U remain in the wetland, mostly in five hot spots. The furthest hot spot (9 ha) was 8 km downstream of the source term and accounted for 11% of the detected U. Uranium soil concentrations in this hot spot were as high as 2000 mg/kg and were near perfectly correlated to organic matter and iron concentrations. A hydrological and contaminant transport model was calibrated and validated against measured data. It showed that the hot spots are located only in marshy wetlands, as opposed to uplands, and in areas where stream energy is or was extremely low, such as former ponds. Modeling results suggest that stream particles are responsible for much of the U transport in this system. Surprisingly, few U-rich particles could be found in sediments recovered from the hot spots using autoradiography followed by SEM/EDX techniques. The few hot particles that were found contained 12 to 16 wt% U. Together these results demonstrate that wetlands can be highly effective at immobilizing U for more than 50 years. Furthermore, contaminant reconcentration occurs only in areas where the hydrological conditions as well as sediment biogeochemical conditions are conducive. Results from this meter-to-hectare scale study are being combined with on-going laboratory gram-scale and spectroscopic molecular-scale studies to inform a model to predict water quality in wetlands.

Effect of Organic Ligands on U and Fe Biogeochemistry in Wetland Sediments

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Project: Argonne Wetland Hydrobiogeochemistry Science Focus Area

Project Website: https://ess.science.energy.gov/anl-wetland-sfa/
https://www.anl.gov/bio/project/subsurface-biogeochemical-research

Project Abstract: The Argonne SFA (*Wetland Hydrobiogeochemistry*) studies the processes that govern elemental cycling and particle formation/transport at a DOE field site, the Tims Branch wetland at the Savannah River Site. The organic-rich sediments in this riparian ecosystem experience changing redox conditions that induce transformations of the major elements (C, Fe, P, S), as well as of several contaminants discharged during past operations at the site (Ni, Cr, Zn, Pb, U). Although laboratory studies have isolated some of the effects of redox transformations on speciation, unexpected behavior is sometimes observed in complex natural systems due to unanticipated interactions between the multiple constituents. We characterized a number of intact sediment cores by synchrotron x-ray spectroscopy to determine the elemental distribution and the speciation of Fe and U with depth. The valence of U was dependent on local saturation state. We found U(IV) predominantly in hydrated sediments, indicating the establishment of reducing conditions due to microbial activity. U was present in a form different from synthetic nano-uraninite (UO_2), indicating a significant influence of minerals and organic ligands on the speciation of U(IV) in wetland sediments. To better understand the effects of each, we carried out U(VI) bioreduction experiments with added clay minerals and/or organic ligands (citrate, EDTA, DFOB). Addition of clays alone did not change U(IV) speciation (i.e., uraninite formed). The presence of citrate resulted in a soluble U(IV) complex under all tested conditions. EDTA and DFOB also formed soluble U(IV) complexes, but in systems with Fe-containing clays, the U(IV) complex remained in the solids by interlayer uptake or as a bridging ternary complex. These results illustrate the intricate interdependencies between the constituents of contaminated sediments and provide information for the inclusion of corresponding reactions in transport models. Improved mechanistic models in turn lead to better predictions and policy decisions.

Title: **Microbial Response to Root Substrate Addition is Depth Dependent**

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Project: Belowground Biogeochemistry SFA (lead: LBNL)

Project Websites: https://eesa.lbl.gov/projects/terrestrial-ecosystem-science/

https://tes.lbl.gov/

Project Abstract:

The subsoil (<30 cm) contains almost half of the soil organic carbon (SOC) stock in the top meter of soil (Jobbágy & Jackson 2000, Balesdent et al. 2018), yet most studies only focus on surface layers (Yost & Hartemink 2020). Subsoil temperatures are projected to increase at a similar rate to air and surface soil temperatures (Soong et al. 2020), which can make this deep, relatively stable SOC pool vulnerable to increased microbial decomposition. Nonetheless, there is still no clear consensus on the factors that drive warming-induced changes in SOC stocks (van Gestel et al.2018). To understand the capacity of subsoil to store SOC with climate change, we must understand how decomposition changes with depth and warming.

We examined *in situ* litter decomposition by adding ^{13}C-labelled fine roots to surface (10-14 cm), mid- (40-44 cm), and deep soil layers (85-89 cm) of a coniferous temperate forest in soil classified as alfisols. At our site, we have warmed soil by 4°C relative to control temperatures to 100 cm since 2013. We recovered the root-derived C in bulk soil and microbial phospholipid fatty acids (PLFA) after 1 and 3 years of incubation. The overall recovered litter fraction in bulk soil significantly decreased by 60% in the surface and by 90% in the mid- and deep soil layers from 2017 to 2019, indicating that microbes in the subsoil relied on the added root-C more than surface microbes. Overall, total PLFA significantly decreased with depth (p-value <.0001), corroborating previous work at our site showing a significant decrease in microbial biomass with depth (Zosso et al. 2021). Though the root addition treatment did not significantly change total PLFA, it was on average higher at 85-89 cm relative to the disturbance control. Root addition significantly increased the relative abundance of fungi at 85-89 cm relative to the rest of the soil profile, contrasting previous findings that fungal biomarkers that relied on the added root substrate were less abundant at depth (Hicks Pries et al. 2018). Microbes in subsoil preferentially used the added substrate during the incubation period, leading to an increase in the fungal relative abundance at

depth. Our results suggest that particulate SOC in subsoil could be vulnerable to increased microbial decomposition, which can be exacerbated by warmer soil temperatures (Soong et al. 2021).

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Title: Linking microbial functional traits and organic matter chemistry to identify the pathways of carbon loss in response to warming through the soil profile

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Project: Belowground Biogeochemistry SFA (lead: LBNL)

Project Websites: https://eesa.lbl.gov/projects/terrestrial-ecosystem-science/
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Project Abstract: The microbial mechanisms controlling soil organic matter (SOM) decomposition and its responses to warming are poorly understood, particularly in subsoils, which contain over 50% of global soil carbon. Our prior work has shown that 4.5 years of whole-profile soil warming at a coniferous forest consistently stimulated CO_2 emissions and microbial growth rates at depths down to 1 m, while it decreased plant inputs. Warming only led to net carbon losses from subsoils, although depth-dependent changes in microbiome composition, SOM chemistry, and decomposition of distinct SOM fractions suggests that the microbial mechanisms driving SOM transformation and carbon fluxes are depth-dependent. Microbiomes in deeper soils have different functional traits than those at the surface, namely lower growth rates, carbon use efficiencies and ability to degrade complex carbohydrates, and exoenzymes with different kinetic properties.

We hypothesized that interactions between thermodynamic constraints dependent on SOM composition and microbial life strategies results in CO_2 emissions driven by distinct metabolisms and mechanisms of response to warming through the soil profile. To evaluate this, we are investigating the dynamics of microbial trait distributions and expression, and SOM composition in our whole-soil profile warming experiment using a multi-omics approach. Initial results from 21T-FT-ICR-MS showed that average oxidation states of carbon decreases with soil depth, with a predominance of lignins, tannins and condensed hydrocarbons at the surface, and lipids, proteins, amino-sugars and unsaturated hydrocarbons in deeper soils. After six months, warming led to depletion of more oxidized carbon compounds in surface soils and to their enrichment at mid-depths. However, 4.5 years of warming led to an increase in more oxidized compounds across all depths, possibly due to accumulation of tannins and other aromatic compounds, rather than more easily degradable carbohydrates. Interestingly, ethanol and methanol were the most abundant compounds quantified by ^{1}H-NMR, with relatively high concentrations through the soil profile, whereas those of more thermodynamically favorable compounds (glucose, acetate, and glycerol) declined sharply with depth. Consistently, we identified enzymes involved in alcohol, including

methanol, metabolism in the metaproteomes, as well as in carbon monoxide, carboxylic acid, and alkane oxidation, further supporting a role for simple carbon compounds in carbon fluxes, beyond biomass depolymerization.

These results suggest that variation in SOM composition with depth and during warming may constrain the metabolisms driving carbon fluxes, and that feedbacks between different microbial life strategies and substrate-dependent thermodynamics may be key regulators of carbon budgets in response to warming through the soil profile.

Title: **Association Between Soil Organic Carbon and Calcium in Acidic Grassland Soils from Point Reyes National Seashore, CA**

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Project: Berkeley Lab Belowground Biogeochemistry SFA (LBNL)

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Project Abstract: Organo-mineral association and complexation processes are important for the retention and accumulation of soil organic carbon (SOC). Most of the research into these processes has focused on the biogeochemical interactions between SOC and Fe or Al, largely overlooking a role of Ca. Recent studies have demonstrated a strong link between calcium (Ca) and soil organic carbon (SOC) in a range of soil types (Rasmussen et al., 2018; Rowley et al., 2021; Yang et al., 2020), but a current paradigm suggests that Ca-mediated accumulation of SOC is predominantly constrained to soils with carbonates (pH > 6; Rowley et al., 2018).

To investigate the role of Ca in SOC accumulation of acidic soils, we combined classical characterisation and synchrotron-based spectro-microscopic methods to analyse three soil cores taken from grasslands with a pH gradient (soil pH 3.8 - 5.3) at the Point Reyes National Seashore, California. Bulk soil samples were characterised in detail, measuring classical soil physical (texture), mineralogical (X-ray diffraction), and chemical properties (pH, SOC, exchangeable and total elements). Subsequently, bulk Ca K-edge spectra were obtained for the core samples at three depths. We also used microprobe-coupled μ-X-ray absorption spectroscopy (μ-XANES; Ca K-edge) and STXM (Ca L-edge and C K-edge) to investigate the bonding environment of Ca and C in our samples, and their association with other elements (Al, Fe, K, Mg, Na, P, S, and Si).

Both the Ca and SOC content were high in our samples and were correlated in multivariate analyses of our standard characterisation dataset. Linear combination fitting of the bulk Ca K-edge XANES data revealed that Ca was predominantly associated with organic matter at our site. Additionally, STXM analysis showed that Ca had a strong spatial correlation with C, presenting a

higher spatial correlation than C with Fe. In characterising the SOC, we demonstrated that C associated with Ca had higher peaks in the alkyl and aromatic regions of the C K-edge spectra, relative to C associated with Fe or Fe-Ca-C. These spectral features are consistent with published spectra of C with a lignin-like nature and were observed in samples obtained from up to 70 cm depths. It therefore seems that Ca-C association is linked to the preservation of more plant-like products, even at depth in acidic grassland soils with no carbonate, potentially challenging existing paradigms (Rowley et al., 2018) that these Ca-mediated processes are only found in soils with a pH > 6.5.

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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.

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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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Project Website: watershed.lbl.gov

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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BER Program: ESS

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.

Biogeochemistry of the Pond B Water Column, Savannah River Site, South Carolina

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Project: LLNL DOE SFA: BioGeoChemistry at Interfaces
Project Website: https://ess.science.energy.gov/llnl-actinides-sfa/

Pond B at Savannah River Site (SRS) is an ideal location for examining the biogeochemical cycling of Fe, Pu, organic matter, and other metals in a monomictic stratified pond. This pond received reactor cooling water from 1957–1964 containing trace levels of radionuclides. Since then, Pond B has remained relatively isolated except for a few studies conducted in the late 1980s, which demonstrated Pu cycling with seasonal anoxia.

During summer thermal stratification, aqueous concentrations of Pu, Fe and ^{137}Cs increase with depth coupled with anoxia, low Eh, and high suspended solids, likely linked to reductive dissolution of Fe-(oxy)hydroxides and mobilization of organic matter. These trends are consistent with 1983 measurements of ^{239,240}Pu and ^{137}Cs activities in Pond B, although Pu and decay-corrected ^{137}Cs activities have since decreased 2- to 3-fold in the water column. Pu isotopic ratios in water samples are consistent among all locations and depths and are similar to ratios of upstream sediments, suggesting that Pu in the pond is dominantly from historical releases and not atmospheric fallout.

The microbial community was also examined to understand biotic mechanisms that impact Pu and Fe cycling. We observed that during stratification, the Pond B water column microbiome varies with depth rather than spatial location and can be broadly categorized by the three distinct stratification layers. Metal (e.g., iron) oxidizers/reducers were prevalent during stratification, likely influencing Pu immobilization onto Fe-(oxy)hydroxides in the thermocline and Pu mobility/reduction in the deep, anoxic layer. Notably, Fe(II) oxidizers were most abundant in the hypoxic/anoxic zones, while Fe(III) reducers dominated the deep, anoxic layer. In contrast to summer stratification, during spring turnover, the microbiome is homogenized throughout Pond B, reflecting the uniform geochemistry (e.g., oxygen concentrations, temperature, metals).

We also observed a shift in the distribution and abundance of organic molecules (dissolved organic matter; DOM) with depth and location. Multivariate analysis based on bulk molecular parameters and relative abundance of individual elemental formulas showed that the molecular composition of DOM was highly stratified and could be separated into three distinct layers in the summer. Surface layer samples were characterized by higher nominal oxidation state of carbon, H/C, and aliphatic compounds. In contrast, the deep anoxic zone was characterized by higher DBE (double bond equivalent), DBE/O, aromatic index, and CRAM (carboxyl rich alicyclic molecules), indicating that the DOM in the deep layer was more refractory.

Factors Controlling Pu-239 and Cs-137 Mobility in Contaminated Isolated Pond Sediments, Savannah River Site, South Carolina

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There remains a lack of knowledge regarding ecosystem transfer, transport processes, and mechanisms, which influence the *long-term* mobility of ^{239}Pu and ^{137}Cs in natural environments, particularly with respect to how anthropogenic radionuclides interact with natural biogeochemical cycles. Furthermore, monitoring the distribution and migration of trace anthropogenic radioisotopes as ecosystem tracers has the potential to provide insight into the underlying mechanisms of geochemical cycles. This study investigated the distribution of the anthropogenic radionuclides ^{239}Pu and ^{137}Cs, along with total organic carbon, iron and trace element concentrations, and the microbial community in contaminated sediments of Pond B at the Savannah River Site (SRS) in South Carolina.

Pond B received SRS R-reactor cooling water from 1957–1964, resulting in trace amounts of ^{239}Pu and ^{137}Cs being introduced into the pond. Since then, the pond has been relatively isolated except for a sampling campaign in the 1980s evaluating radionuclide distributions in the water and sediment. In this work, sediments were collected throughout the Pond B site to determine the spatial variability of Pu and Cs, as well as sediment cores to determine the concentrations of 239Pu, 137Cs, and major and minor elements in the solid phase. Additionally, an electrochemical method using an in-situ core probe was used on wet cores before extraction to determine the concentration and speciation of dissolved redox-active species.

More than 50 years after deposition, ^{239}Pu and ^{137}Cs concentrations in Pond B sediments are primarily located in the upper 5 cm of sediment in an area where deposition of particulate-bound contaminants was most prevalent and located between 5 and 10 cm in areas of high sedimentation. An analysis of the geochemical data coupled with a factor analysis demonstrated different sediment facies across the pond which result in a range of geochemical processes controlling the accumulation of Pu and Cs in the sediment. The highest concentrations of ^{239}Pu and ^{137}Cs appear to be controlled by particulate input from the influent canal. Elevated ^{239}Pu concentrations in the sediments were observed in areas with high organic matter content and high sedimentation rates indicating strong association of Pu with organic matter. Notably, the sediment microbial community at the pond outlet is likely involved in organic matter degradation processes and may impact Pu-associated organic matter.

Plutonium Distribution among Acidic Processing Waste at the Hanford Site, USA: Implications to Long-Term Subsurface Migration

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Between 1955 and 1962, 4 million liters of plutonium (Pu) reprocessing waste from the Plutonium Finishing Plant at the Hanford Site, containing an estimated 50-140 kg Pu, were pumped into the sediments of the 216-Z-9 (Z-9) trench. The waste consisted of high salt (~ 5M NO_3^-, ~ 0.6M Al^{3+}), acidic (pH ~ 2.5) solutions, that also contained the organic solvents: CCl_4, TBP, DBBP, and lard oil. While most of the Pu was observed to precipitate within the first several centimeters,[1] a small fraction of Pu has been detected in the vadose zone at depths of 37 m.[2] The mechanisms controlling Pu migration beneath the trench are unknown. In this study, a series of binary and ternary batch experiments were used to determine Pu partitioning behavior between aqueous, organic, and solid phases representative of the waste constituents and natural sediments of the Z-9 trench. The Pu partitioning behavior observed in the binary and ternary experiments was then used to develop a conceptual model for the transport of Pu in the subsurface.
Our results show that Pu can migrate as a Pu-TBP-nitrate complex in the presence of a TBP-containing organic phase under low pH and high nitrate conditions. Reducing the nitrate concentrations or increasing the pH will lead to Pu partitioning into the aqueous phase and subsequent sorption to native Hanford sediments. Our findings suggest that Pu migration in the subsurface is likely controlled by weak sorption of aqueous Pu under acidic conditions as well as with the formation of Pu-TBP-nitrate complexes in the organic phase. Dispersion of the nitrate plume and the transient nature of the low pH conditions will limit long-term Pu mobility beneath the trench.

1. Ames, L. L. Characterization of Actinide bearing soils: Top sixty centimeters of 216-Z-9 enclosed trench; Richland, WA, **1974**.
2. Cantrell, K. J.; Riley, R. G. A review of subsurface behavior of plutonium and americium at the 200-PW-1/3/6 operable units; **2008**.

Elucidating Coupled Solute Transport, Transformation, and Ecosystem Processes in River Corridors using Stream Tracers

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BER Program: ESS

Project: Critical Interfaces Science Focus Area (Oak Ridge National Laboratory)

Project Website: https://www.esd.ornl.gov/programs/rsfa/

Project Abstract: Metabolically active transient storage zones in stream ecosystems, most notably the hyporheic zone, are ecological and biogeochemical hotspots that exert control over geochemical and metabolic processing and regulate the distribution and transformation of matter and energy in river systems. Multiple natural and anthropogenic factors, including channel morphology, dynamic hydrology, and modifications to nutrient regimes, drive changes in the solute transport dynamics and reactivity of transient storage zones over time and space, which should, in turn, influence rates of whole-stream ecosystem functions such as metabolism and both assimilatory and dissimilatory nutrient transformations. However, there remains uncertainty about the coupling between solute transport, transient storage, and stream ecosystem function within streams, and the relative importance and organization of these coupled processes across systems and watershed scales. Additionally, we lack understanding about the relative importance and organization of these coupled processes across systems and watershed scales. Improving the representation of these coupled processes in both our conceptual and numerical models is essential to developing a more robust predictive understanding of functioning within river corridors. Here, we present insights gained from stream tracer experiments employed across a range of lotic systems to evaluate transient storage and aerobic respiration in relation to varied spatio-temporal patterns in stream structural controls and ecosystem processes. We also summarize new forward modeling capability and uncertainty-aware model-based interpretation approaches that leverage results from the stream tracer experiments. We identify challenges, opportunities, and new experimental approaches for expanding our process understanding across systems and scales and linking this understanding to reach-scale simulations of transport and transformation.

Understanding Environmental Controls on the Composition, Function, and Cycling of Mercury within Fluvial Periphyton

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Project: Critical Interfaces Science Focus Area (Oak Ridge National Laboratory)

Project Website: https://www.esd.ornl.gov/programs/rsfa/

Project Abstract: Periphyton biofilms are complex assemblages that consist of algae, bacteria, fungi, detritus, extracellular polymers, invertebrates, and mineral particles. These complex biofilms play an integral role in stream ecohydrology as they are control points for ecosystem respiration, primary productivity, and organic matter cycling, while providing an important food source for higher trophic position organisms. Identifying the environmental physicochemical factors (e.g., disturbance regime, nutrient concentrations) that contribute to observed variability in fluvial biofilm community structure and function is needed for developing predictive models of stream biogeochemistry.

One poorly constrained biogeochemical function of fluvial biofilms is the production of monomethylmercury (MMHg) from inorganic mercury (Hg). Fluvial periphyton communities host the active anaerobic microbes capable of the microbially-catalyzed production of MMHg due to the steep geochemical gradients between fully oxic and anoxic conditions within these biofilms. Controlled laboratory experiments have demonstrated that actively photosynthesizing biofilms may generate a significant fraction of the MMHg flux in East Fork Poplar Creek (EFPC), a Hg contaminated creek in Oak Ridge, TN.

To better understand the relationship between environmental physicochemical factors and periphyton biofilm composition and function, we are conducting in-stream experiments within EFPC across multiple seasons to control for temporal variability. Utilizing a natural gradient of nutrient concentrations between two locations within EFPC, we can determine functional characteristics of biofilm colonized under relatively lower and higher nutrient concentrations, as well as assess the impacts of altering the nutrient regime to which an established periphyton community is exposed via physical translocation between locations. The resulting biofilms are then used in experiments to quantify measures of function (Hg methylation and MMHg demethylation kinetics, production of thiol-containing biomolecules) and community composition

(16s, 18s, ITS, and *hgcA* sequencing). Application of our transient availability model, developed for quantifying Hg methylation kinetics in biofilms, to biofilms grown under experimental treatments of varying length will allow us to quantify the impact of seasonally variable physicochemical factors on periphyton methylation rates. Sequencing data will be utilized to evaluate the relative impacts of community structure and interaction within the periphyton microbiome that drive variations in observed rates of Hg transformation. By providing insights into the environmental controls on the community composition and function of complex fluvial biofilms, this work aims to inform future research into the critical ecosystem processes in river corridors impacted by the activity of periphyton assemblages.

Linking Trace Metal Biogeochemistry and Carbon-Nutrient Cycling: The Role of Metallophores

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Project: Critical Interfaces Science Focus Area (Oak Ridge National Laboratory)

Project Website: https://www.esd.ornl.gov/programs/rsfa/

Project Abstract: Metal ions are essential components of metalloenzymes, which drive many biogeochemical carbon and nutrient cycles at the molecular scale. Microorganisms have developed strategies to overcome potential trace metal limitations by utilizing metallophores to facilitate the efficient uptake of trace metals. Thus, metallophores assume a significant role in controlling the bioavailability of trace metals. Metalloenzymes catalyze many key reactions driving critical metabolic processes, and they work at the interface between the cycling of trace metals and macronutrients, such as carbon and nitrogen. Methanobactin, a small peptide produced by some methanotrophs, is an example of a metallophore involved in copper (Cu) acquisition by methanotrophic bacteria linking the trace metal copper to the cycling of carbon (methane) in the environment. Additionally, methanobactins are known to form strong complexes with other transition metals, such as Hg, Zn, and Cd, affecting their biogeochemical transformations and bioavailability.

In this work, we present several case studies, such as discoveries of two novel methanotroph strains, *Methylomomas* sp. strain EFPC1 and *Methylococcus* sp. strain EFPC2, isolated from East Fork Poplar Creek, a Hg-contaminated stream in Oak Ridge, Tennessee, and interspecies interactions among methanotrophs. We show that some methanotrophs lacking genes for methanobactin biosynthesis are not limited for Cu by utilizing methanobactins produced by others. Certain methanobactins are also found to enhance the rate and efficiency of Hg methylation by the mercury-methylating bacteria, *D. desulfuricans* ND132 and *G. sulfurreducens* PCA, due to the formation of Hg-methanobactin complexes. We also investigate the interplay between solution-phase configurations, metal interactions and the spectroscopic signatures of methanobactin-metal complexes. Our results represent the first combined computational and experimental spectroscopy study of methanobactins and shed new light on molecular interactions and dynamics that

characterize complexes of methanobactins with Group 12 transition metals. Collectively our results underscore the complex roles of exogenous metallophores produced by microbes in controlling bioavailability and biogeochemical transformation of metals, which in turn exert a modulating influence on carbon and nutrient cycling in the environment.

Effects of Coupled Biogeochemical Processes on Soil Organic Carbon Storge and Fluxes

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Project Abstract: Improved understanding of the biogeochemical processes that regulate decomposition of organic matter and their incorporation into process-based models are needed to predict how watersheds will store and process carbon (C) in response to changing climate. Current ecosystem representations focus largely on biological components and disregard geochemical processes; however, soil carbon storage and fluxes are regulated by complex biotic and abiotic interactions amongst organic matter, nutrients, and metals. The objective of this research is to use laboratory, field, and modeling experiments to investigate interactive effects of manganese (Mn), nitrogen (N), and warming on leaf litter decomposition and organo-mineral interactions. Dissolved Mn stimulates enzymatic oxidation of recalcitrant lignin by soil microorganisms and may serve as a limiting nutrient to decomposition. Furthermore, Mn enrichment has been proposed to counteract inhibitory effects of N deposition on decomposition rates.

In a field decomposition experiment, surface organic soils were enclosed in nylon mesh bags and incubated for up to one year in upland soils of the temperate forested Walker Branch watershed in east Tennessee. Soils were either warmed +2-3°C or not and received between zero to 10 mg g^{-1} monthly aqueous Mn(II) addition. Measurements of litter mass loss and soil respiration were coupled with spectroscopic measurements and microbial analyses to evaluate C transformation and efflux during decomposition. Complimentary laboratory incubations were performed to measure the effects of Mn enrichment on C transformation and greenhouse gas (CO_2, N_2O) production in N-fertilized and unfertilized agricultural soils. We further developed a novel biogeochemical model based on existing observations that simulates how Mn bioavailability interacts with N and warming to influence soil organic C stocks in temperate forests. We determined that Mn addition accelerated decomposition of leaf litter into CO_2 and into decomposition products that associated with minerals, and these effects were primarily observed under experimental N enrichment. Mn addition also suppressed N_2O emissions, indicating the potential for complex effects of Mn biogeochemistry on greenhouse gas emissions. Based on simulations and experiments, we predict that warming and N enrichment generate Mn limitation

to litter decomposition where Mn is poorly soluble, enabling C accumulation over decadal timescales. Through this work, we aim to establish a quantitative coupled modeling-experimental framework for evaluating geochemical controls on how C is stored, processed, and released from watersheds.

Machine Learning Model Prediction of Streamflow in Walker Branch Watershed

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Project: Critical Interfaces Science Focus Area (Oak Ridge National Laboratory)

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Project Abstract: How will the hydro-biogeochemical function of watersheds respond to hydrologic intensification and land use/land cover change from local to regional scales? Addressing this question is crucial but also challenging. It requires large data, comprehensive model representation, and sophisticated data-model integration. Although a broad collection of diverse observations is increasing, current hydro-biogeochemical models have inadequate watershed process representation, and existing data assimilation methods are not powerful enough to incorporate diverse data for prediction.

Here we highlight the use of machine learning (ML) methods for hydro-biogeochemical simulations. ML models are powerful in extracting patterns, discovering new knowledge from multi-scale, multi-types of data, and identifying underlying cause-effect relationships for predictive understanding. We applied a ML approach, called Long Short-Term Memory (LSTM) network, to understand rainfall-runoff processes using data collected in Walker Branch Watershed (WBW). WBW is a 97.5-ha, temperate deciduous forest watershed located in East Tennessee, USA. Hydrological, biogeochemical, and ecological process studies have been carried out in this seminal research catchment since 1967. The multiple, long-term datasets that have been collected in WBW provide the opportunity to apply ML methods to predict hydrological dynamics. These long-term datasets include daily climate and soil temperature (1993-2010), precipitation (1969-2012), streamflow (1969-2014), and stream chemistry (1989-2013). We use LSTM to simulate streamflow based on meteorological and environmental observations including precipitation, air temperature, relative humidity, and soil temperature. A total of 14 years of daily data (1993-2006) were used, with the first 10 years for network training and the remaining 4 years for out-of-sample prediction. Results indicate that LSTM performed well in the training period where its predictions closely matched observed streamflow with the Nash-Sutcliffe efficiency of 0.97, although the predictions were relatively poor in 2004 and 2006. After hypothesis testing, we found that the poor performance in these two hot and dry years resulted from the lack of ET-related observations that were not included in the training and thus the relevant processes were not learned.

Here we used an interpretable LSTM which not only calculates variable importance but can also guide data collection and model development. We are working on ML model uncertainty quantification and will use the uncertainty bounds to indicate when the ML results can be trusted in the projection of future streamflow. Additionally, we are developing hybrid ML models to sufficiently leverage the data information and our domain knowledge for improving predictions.

ORNL Terrestrial Ecosystem Sciences SFA Abstracts
for the 2022 ESS PI Meeting

Overview Poster Abstract

Hanson PJ and Ricciuto DM **ORNL's Terrestrial Ecosystem Science – Scientific Focus Area (TES SFA): a 2022 Overview**

Spark Presentation Abstracts (x10)

1. Salmon VG et al. – **Five Years of Experimental Manipulations at SPRUCE: Consequences for Nutrient cycling in Vegetation & Peat**
2. Weston DJ et al. – **An alternative to adapt, migrate or die: insights into microbial enhanced plants resilience to warming**
3. Roth S et al. – **Microbial Community Responses to Elevated Temperature and CO_2 in Peat Decomposition Ladders**
4. Mao J et al. – **Above- and Belowground Phenology Modeling of ELM Using the SPRUCE Observations**
5. Gu L et al. – **Coupling Photophysics, Photochemistry, and Biochemistry for a Complete Mechanistic Modeling and Remote Sensing of Photosynthesis**
6. Wood JD et al. – **From Below- to Aboveground, and Integrated Ecosystem Drought Responses**
7. Abramoff RZ et al. – **Modeling Climate Sensitivity of Above and Below Ground Processes at MOFLUX**
8. Warren J – **Dynamic Imaging of Root and Rhizosphere Processes**
9. Craig ME et al. – **Evaluating and Modeling the Alternative Hypotheses that Connect Organic Inputs to Soil Carbon**
10. Wang B et al. – **Taming fine-root systems complexity to reduce Earth System Model uncertainty**

ORNL's Terrestrial Ecosystem Science – Scientific Focus Area (TES SFA): a 2022 Overview

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Project: ORNL Terrestrial Ecosystem Science Scientific Focus Area (TES SFA)
Project Websites: http://mnspruce.ornl.gov; http://tes-sfa.ornl.gov

Understanding fundamental responses and feedbacks of terrestrial ecosystems to climatic and atmospheric change is the aim of the Terrestrial Ecosystem Science Scientific Focus Area (TES SFA). Improved predictive knowledge of ecosystem dynamics is the long-term motivation for our research. Overarching science questions are:

1) How will atmospheric and climate change affect the structure and functioning of terrestrial ecosystems at spatial scales ranging from local to global and at temporal scales ranging from sub-annual to decades and centuries?
2) How do terrestrial ecosystem processes, and the interactions among them, control biogeochemical cycling of carbon and nutrients, the exchanges of water and energy, and the feedback to the atmosphere, now and in the future?

The proposed science includes manipulations, multi-disciplinary observations, database compilation, and fundamental process studies integrated and iterated with modeling activities. The centerpiece of our climate change manipulations is the Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment that tests multiple levels of warming at ambient and elevated CO_2 on the vegetation response and biogeochemical feedbacks from a *Picea-Sphagnum* ecosystem. Other efforts aim to improve mechanistic representation of processes within terrestrial biosphere models by furthering our understanding of fundamental ecosystem functions and their response to environmental change. The TES SFA integrates experimental and observational studies with model building, parameter estimation, and evaluation to yield reliable model projections. This integrated model-experiment approach fosters an enhanced, interactive, and mutually beneficial engagement between models and experiments to further our predictive understanding of the terrestrial biosphere in the context of Earth system functions.

Five Years of Experimental Manipulations at SPRUCE: Consequences for Nutrient cycling in Vegetation & Peat

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Ombrotrophic peatlands store over a thousand gigatons of soil carbon (C) but primary productivity of these ecosystems is constrained by low availability nitrogen (N) and phosphorus (P; Bridgham et al., 1996; Nichols & Peteet, 2019). Elevated temperatures and an increase in atmospheric CO_2 may stimulate of peatland soil C, especially in northern peatlands (Crowther et al., 2016). Plant growth under climate change may offset some of these C losses but will depend on the balance of N and P availability versus to plant demand for these nutrients. At the SPRUCE experimental site, three years of warming increased losses of C from the ecosystem at a rate of 31.3 gC m^{-2} y^{-1} (Hanson et al., 2020) while availability of N and P in peatland soils increased dramatically (Iversen et al. *In Press*). This prompts the question: Are plants at SPRUCE utilizing the newly available N and P? We compiled comprehensive N and P budgets for bog vegetation following five years of experimental warming and elevated CO_2 to determine the answer. Annual tree surveys at SPRUCE were used to calculate aboveground tree biomass and net primary productivity (NPP) while understory aboveground biomass NPP were determined based on clip-plots. Ingrowth cores were used to quantify NPP of fine roots of all plant functional types (Malhotra et al., 2020). Biomass and NPP of *Sphagnum* moss was based on percent cover surveys and growth in mesh columns (Norby et al., 2019). Species-specific N and P content of plant tissues were measured and applied to vegetation pools and fluxes. Since peat stores approximately 99 and 98% of the ecosystem N and P pools at this site (Salmon et al., 2021), we decided to also assess whether there were detectable changes in peat N and P stocks or stoichiometry at SPRUCE based on peat profiles collected in 2012 and 2020. Preliminary results from this analysis indicate the decline of *Sphagnum* in warmed plots has greatly reduced the storage of N and P in moss biomass but the manipulative treatments have had little impact on tree biomass N and P stocks. Acrotelm peat within hollows at SPRUCE has altered N storage due to a significant interaction between warming and elevated CO_2 treatments. These results indicate that vegetation within an ombrotrophic bog experiencing 5 years of simulated climate is slow to take advantage of increased N and P availability, potentially leading to loss of nutrients from the ecosystem.

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An alternative to adapt, migrate or die: insights into microbial enhanced plants resilience to warming

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The onset of changing climatic conditions is eliciting research in the resilience of ecosystems to challenging environmental conditions. Initial results from such studies have led to the generalization that many plant species will have to either adapt or migrate in order to avoid extinction. However, species interactions, such as those mediated by microbes may provide an alternative approach. Here, we use a microbiome transfer approach to test if microbiome thermal origin influences host plant thermotolerance. We leveraged an experimental whole-ecosystem warming study to collect field grown *Sphagnum*, mechanically separate the associated microbiome and then transfer onto germ-free laboratory *Sphagnum* for temperature experiments. Host and microbiome dynamics were assessed with growth analysis, chlorophyll-*a* fluorescence imaging, metagenomics, metatranscriptomics, and 16S rDNA profiling. Microbiomes originating from warming field conditions imparted enhanced thermotolerance and growth recovery at elevated temperatures. Metagenome and metatranscriptome analyses revealed that warming altered microbial community structure in a manner that induced the plant heat shock response, especially the Hsp70 family and jasmonic acid production. The heat shock response was induced even without warming treatment in the laboratory, suggesting that the warm-microbiome isolated from the field provided the host plant with thermal preconditioning. Our results demonstrate that microbes, which respond rapidly to temperature alterations, can play key roles in host plant growth response to rapidly changing environments.

Microbial Community Responses to Elevated Temperature and CO_2 in Peat Decomposition Ladders

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Peatlands are ecosystems in which plant primary production has historically outpaced microbial decomposition and, as a result, peatlands store approximately one-third of the global terrestrial organic matter. As climate change accelerates, increased temperature and atmospheric CO_2 have the potential to alter the processes involved in organic matter accumulation and degradation. Specifically, warming may influence microbial communities involved in organic matter decomposition, leading to increased decomposition and further production of the greenhouse gases CO_2 and CH_4. To investigate how increased temperature and elevated CO_2 may impact microbial communities associated with organic matter decomposition, we utilized the Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment in northern Minnesota. Peat decomposition ladders consisting of known quantities of peat in discrete mesh bags were placed into the SPRUCE treatment chambers at four depths below the surface of the peat in 10 cm increments (between 0-40 cm) allowing them to decompose *in situ* and were collected after three years. Peat mass loss and carbon:nitrogen (C:N) changes were quantified, and characterization of the microbial communities were accomplished through 16S rRNA (bacterial/archaeal) and ITS (fungal) amplicon sequencing. Our results show that microbial community composition is significantly impacted by depth, temperature, and CO_2 treatment. We found that bacterial/archaeal and fungal alpha-diversity were highest near the surface (0-10 cm) and in the plots with the highest warming treatment (+9° C). Numerous microbial phyla were significantly differentially abundant between temperature treatments, indicating selection of specific microbes with warming. We did not find a significant correlation between microbial community composition and peat mass loss or C:N. This may be due to a lag between community shift and decomposition process responses to warming and our planned outyear collections of peat decomposition ladders will be used to test this hypothesis. Collectively, our results indicate that increased temperature and CO_2 as a result of climate change can alter microbial communities in peatlands, potentially contributing to increased decomposition rates and greenhouse gas emissions.

Above- and Belowground Phenology Modeling of ELM Using the SPRUCE Observations

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Vegetation phenology controls the seasonal cycle of land surface properties and determines the exchange of energy, water, and carbon fluxes between the land and the atmosphere. To date, the phenology representations in land surface models rarely distinguish between the above- and belowground phenology; and this approach has been demonstrated to be unrealistic by many observational studies, especially for the boreal region, where the belowground growing season can be considerably longer and have different environmental cues than the aboveground season. This study continues previous phenology development effort of the land model of the US Department of Energy's Energy Exascale Earth System Model (ELM of E3SM) using the Spruce and Peatland Responses Under Changing Environments (SPRUCE). In addition to updating the leaf phenology of boreal evergreen needleleaf trees based on ground phenology observations, this study examined multiple formulas, fitted using minirhizotron-observed root growth data, for the belowground phenology of various plant functional types (e.g., boreal evergreen needleleaf and deciduous needleleaf trees, boreal deciduous shrubs). Different combinations of above- and belowground phenology algorithms were further intercompared by evaluating the simulations against selected SPRUCE observations (e.g., leaf area index, water outflow, soil carbon fluxes, and their temperature responses). The updated ELM, which contains the best set of phenology scheme, showed superior performances compared to the original ELM, demonstrating the importance of accurate presentations of above- and belowground phenology in land surface models.

Coupling Photophysics, Photochemistry, and Biochemistry for a Complete Mechanistic Modeling and Remote Sensing of Photosynthesis

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Photosynthesis consists of light and carbon reactions. The light reactions can be further divided into the photophysical and photochemical reactions because these two groups of reactions are spatially separated, follow different laws, and operate at vastly contrasting time scales. Recently, we have successfully developed steady-state, mechanistic models for the photophysical and photochemical reactions, respectively. The photophysical model predicts the partitioning of absorbed photon energy among different dissipation pathways. The photochemical model describes the photosynthetic electron transport controlled by the redox reactions between enzyme complexes and electron carriers along the electron transport chain between PSII and PSI. The developed photophysical and photochemical models can be directly coupled with the conventional Farquhar-von Caemmerer-Berry biochemical (carbon reaction) model. This coupling forms a complete model of photosynthesis to predict essentially all light and carbon reaction variables of interest at leaf and canopy scales, such as net and gross photosynthetic rates, actual electron transport rates, state transitions, ratio of cyclic electron transport in PSI, fluorescence emission, redox states of PSII, plastoquinone, and cytochrome b_6f complex, non-photochemical quenching, and constitutive heat dissipation. We have tested the coupled model with pulse amplitude modulated (PAM) fluorometry and gas exchange measurements made on leaves of C_3 and C_4 species collected in the US, Canada, China, the Netherlands, and Finland. The species tested include lianas, shrubs, boreal deciduous trees, boreal evergreen needle-leaf tree, temperate deciduous trees, tropical deciduous trees, tropical evergreen trees, C_3 grasses, C_4 grasses, and different crop varieties.

The coupled photophysical-photochemical-biochemical model advances photosynthesis research in the following aspects:

- The PAM fluorometry and gas exchange measurements, which are the two most important data sources for studying photosynthesis at the leaf level, can now be used jointly in a unified framework for process understanding and carbon cycle model development.
- The relationship between sun-induced chlorophyll fluorescence and photosynthesis can now be simulated fully mechanistically for remote sensing applications.
- Different energy dissipation pathways can be simulated for better understanding land surface energy balance and temperature dynamics.
- Redox states of major enzymes and mobile electron carriers of the electron transport chain can be inferred directly from PAM fluorometry measurements to study state transition and regulation of electron transport and photosynthesis.
- For the first time, state transitions and ratio of cyclic electron transport are formally represented in photosynthesis modeling.
- The model also provides a logical explanation on why all land plants have a thylakoid with grana stacks.

From Below- to Aboveground, and Integrated Ecosystem Drought Responses

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Drought, a pervasive threat to plant productivity across the globe, is projected to intensify under climate change. Accurate representations of plant and ecosystem drought responses are needed for carbon cycle/climate projections to support decision making for adaptation and risk management. While many aspects of plant drought responses are well-understood, there are gaps in mechanisms, methodologies, and data at the scale of whole ecosystems. Specifically, how the dynamics of processes throughout the entirety of the soil-plant-atmosphere continuum aggregate to control ecosystem-level responses and feedbacks to drought of varying intensities and frequencies. To address these gaps, we leverage the unique data sets collected at the Missouri Ozark AmeriFlux (MOFLUX) site, which is situated in a drought-prone *Quercus-Carya* (oak-hickory) forest in the transitional zone between the Eastern Deciduous Forest and the Great Plains. This site experiences frequent seasonal physiological drought, and a broad range of conditions ranging from years with no water stress to exceptional drought. MOFLUX is thus an ideal testbed for observing and modeling drought responses at a range of spatiotemporal scales, and our historical monitoring has emphasized the coordinated collection of ecosystem flux, soil, and ecophysiological data.

Our recent efforts have focused on developing understanding of the coupling of above- and below-ground processes to shed light on how forests respond to drought. Specifically, this has involved the addition of capacity for partitioning soil respiration into heterotrophic and autotrophic component fluxes, the observation of canopy sun-induced chlorophyll fluorescence (SIF) as a direct signal of photosynthesis and augmented measurements of leaf water potentials. Our overall scientific approach has focused on three areas: (i) studying the drought response of soil respiration and its components, (ii) how drought affects the coupling of photosynthesis with soil respiration fluxes, and (iii) developing the theory and testing ecosystem-level drought response traits that can be derived from flux and leaf water potential observations (e.g., a whole-ecosystem wilting point).

This “Spark” talk will provide an overview of these research activities and perspectives on how these empirical analyses can address deficiencies in modeling ecosystem drought responses. Specifically, we will emphasize what we see as the value of ecosystem functional traits for understanding drought responses and how they can be used to better evaluate the performance of models.

Modeling Climate Sensitivity of Above and Below Ground Processes at MOFLUX

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When considering belowground ecosystem responses to climate change, the soil is often treated as a monolith, i.e., considering root and soil microbial respiration together as the total soil respiration flux. However, plant roots and soil microorganisms represent fundamentally different components of belowground ecosystems with different potential sensitivities to drought, temperature extremes, and diurnal, seasonal, and inter-annual changes in productivity.

Together plant roots and soil microorganisms dominate ecosystem carbon (C) losses via respiration but are also responsible for soil C formation and stabilization. Therefore, the future balance of C that is allocated to and remains in soil depends on the relative climate sensitivity of plant productivity and belowground allocation, root respiration, and microbial respiration. We are exploring the climate sensitivity of belowground processes across multiple temporal scales (i.e., diurnal, seasonal, inter-annual), using long-term measurements from the Missouri Ozark AmeriFlux (MOFLUX) site. This heavily instrumented *Quercus-Carya* (oak-hickory) forest is located in the Ozark Border Region of Central Missouri, which experiences seasonal soil water deficits because of high precipitation variability, evapotranspiration, and vapor pressure deficit. The MOFLUX site has measured hourly soil respiration using 8 or 16 automated chambers since 2004, with a subset of chambers over plots where roots were excluded since 2017.

We are identifying quantitative frameworks to partition climate and plant allocation effects on autotrophic and heterotrophic respiration across temporal scales, including statistical and process-based models. The main objective is to decompose the real-time and time-lagged effects of photosynthesis, temperature, and soil moisture on belowground activity. We particularly aim to understand effects of seasonal drought on plant root and microbial activity by exploring mathematical relationships that reflect different hypotheses about the roles of matric potential, diffusion, and oxygen limitation. Modeling frameworks where the structure and key parameters are constrained using long-term measurements can be used to project C responses and their uncertainty to future climate.

Dynamic Imaging of Root and Rhizosphere Processes

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Attenuation-based neutron radiography and computed tomography are currently utilized for the study of plant-soil interactions *in situ*. Results with various woody plants, maize and switchgrass indicate significant variability in water dynamics across the soil-rhizosphere-root pathway, including root water uptake and hydraulic redistribution, hysteresis in water release curves and soil wettability. Measured water extraction rates by cottonwood roots ranged from 0.003 to 0.02 g cm^{-2} root surface h^{-1}, with rates declining for larger roots. Across species, root rhizosphere development increases with root size, stabilizing as roots reach ~2 mm in diameter. Analysis leveraged development of a novel image analysis software to identify and segment roots, and analyze root, rhizosphere, and soil water dynamics. Neutron radiography and paired laboratory measurements have also indicated significant root and mycorrhizal impacts to the soil hydraulic parameters, including hydraulic conductivity and residual water content, and the impacts were more pronounced in sandy soil as compared with silt-loam. While bulk water dynamics are readily visible using neutron radiography, alternate or novel techniques are needed to assess higher resolution water dynamics (e.g., <50 um), symbiotic root-microbial relationships, development of gaps across the rhizosphere that can isolate the root from the soil, and critically, nutrient, ion or exudate uptake or release dynamics.

Evaluating and Modeling the Alternative Hypotheses that Connect Organic Inputs to Soil Carbon

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The rate and quality of carbon inputs to soil are a primary control on belowground carbon storage, and carbon inputs are being altered by environmental changes—e.g., those that alter productivity or shift plant communities. Yet, the ability of soil carbon models to simulate the effects of altered inputs has been repeatedly challenged in recent years. Conventional models predict that soil carbon should increase linearly with input rates, and most dramatically with low-quality inputs. But modern biogeochemical theory emphasizes that microbial and mineral interactions can lead to counterintuitive relationships between inputs and soil carbon. For example, priming effects could offset increased inputs, or fast-decomposing plant products could promote greater mineral stabilization of soil carbon. The newest generation of soil carbon models attempt to capture these phenomena by including more sophisticated representations of mineral and microbial dynamics, yet these models make vastly different predictions because immense uncertainty still exists about the processes connecting inputs to soil carbon.

Here, we discuss our progress on a key question: How do alterations to the rate and quality of organic inputs drive changes in soil carbon storage? We have implemented several microbially explicit models in the multi-assumption architecture and testbed (MAAT)—a modular modeling code that can easily vary model process representations—with the goal of identifying the sources of process-level uncertainty among contemporary soil carbon models. We find that models simulate markedly different responses of soil carbon to alterations in inputs, ranging from highly sensitive to complete insensitivity. Alternative hypotheses about the turnover of mineral-associated and microbial biomass pools account for a large portion of this uncertainty. Whereas both processes are often modeled as a linear first-order process, results from a literature synthesis and from microcosm experiments support the hypothesis that both processes depend on the size of the microbial biomass pool. Standardizing models to include this assumption leads to a convergence of model predictions. We will discuss how using MAAT, or similar tools, to probe process-level uncertainty can inform empirical studies to efficiently progress our predictive understanding of ecosystem carbon cycling.

Taming fine-root systems complexity to reduce Earth System Model uncertainty

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Terrestrial biosphere models are confronted with huge structural and parameter uncertainty. Improving leaf and canopy processes has been the focus since the 1980s. However, the rudimentary representation of fine-root systems forms another large model-data discrepancy. Theoretical and empirical advances in the last two decades have revealed structural and functional differentiation and cooperation within fine-root systems underlying their functioning of nutrients and water acquisition and transport. To close this model-data gap, we propose a 3-pool structure of TAM (Transport, Absorptive, and Mycorrhizal fungi) to model vertically resolved explicit fine-root systems. We hypothesize that TAM will contribute to reducing uncertainty in terrestrial biosphere models. We discuss realization of this TAM structure using an APD scheme (Allocation, Partitioning, and Distribution) in the context of Energy Exascale Earth System Model (E3SM) Land Model (ELM). ELM is representative of existing land surface models grouping heterogeneous fine roots into a single homogeneous pool. Accounting for parametric and structural uncertainty, a demonstration of TAM at two temperate forests (evergreen and deciduous) shows robust impacts of dampening GPP, heterotrophic respiration, and soil carbon stock but of increasing fine-root biomass. TAM captures structural and functional heterogeneity within fine-root systems and provides a framework that can best leverage increasingly explicit root and fungal traits data (e.g., FRED: Fine Root Ecology Database). Though with challenges for a full test of the uncertainty reduction hypothesis, TAM holds promise to guide empirical root ecology, advance understanding of ecosystem functioning, and improve ESMs accuracy. We advocate for its embrace by both modelers and empiricists.

Integrated Modeling of Carbon and Nitrogen Cycling in River Corridors Across the Yakima River Basin

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Project Abstract: *This element of the PNNL SFA seeks to quantify the cumulative impacts of river corridor hydrologic exchange flows (HEFs), dissolved organic matter (DOM) chemistry, and microbial activity on biogeochemical cycling, water quality, and contaminant mobility across the Yakima River Basin (YRB) under both baseline and disturbance conditions.* River corridors play important roles in carbon and nitrogen cycling and removal of excess nutrients. We are developing a new approach to mechanistically represent the river corridor as an integral part of a watershed using unstructured meshing in ATS, seamlessly linking dynamic river flow processes and heterogeneous terrestrial inputs. Leveraging ATS-PFLOTRAN coupled through the Alquimia interface from the IDEAS-Watersheds software ecosystem, we performed coupled hydrologic and biogeochemical modeling at the American River watershed to investigate water, energy, and solute fluxes across the river-groundwater interface in connection to variations in land use, hydrogeology, climate, and disturbances. The biogeochemical hot spots and hot moments within the river corridors are found to be strongly influenced by riverbed properties and flow conditions. SWAT models are set up across the Yakima River Basin (YRB) to study how watersheds respond to wildfires of various burn severity and history. The simulated water quantity and water quality responses (e.g., water temperature, suspended solids, total nitrogen and total phosphorous) are used to guide where we perform sampling and monitoring within the YRB to improve the predictive understanding of fire impact. Machine learning methods have been applied to integrate data from USGS river gauges and remote sensing to improve model parameterization and calibration. By exploring interactions among these three watershed response variables, i.e., streamflow, evapotranspiration and snow cover, for calibrating the ATS model at the American River Watershed, we found that remotely sensed ET data products might provide as useful information as the streamflow for watershed model calibration in cases where stream gage data are unavailable. Our approach can be generalized beyond the YRB and applied to other basins facing environmental disturbances and water challenges of national significance.

Hydrobiogeochemical Variability: Mechanisms Governing Reaction- to Basin-Scale Hydrobiogeochemical Regimes

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Project Website: https://www.pnnl.gov/projects/river-corridor

Project Abstract: *This element of the PNNL River Corridor SFA seeks to identify places/times across the Yakima River Basin (YRB) in which sediment-associated metabolism strongly influences active channel biogeochemistry, and to reveal drivers of underlying molecular properties.* To represent processes governing river corridor biogeochemistry in predictive models, we need to understand how and why biogeochemical contributions from sediment-associated organisms vary through space/time; such contributions vary from 3-96% of respiration. Recent RCSFA work predicts spatial variation in sediment contributions to respiration. To evaluate these predictions, we are deploying sensor systems across 2nd-7th order streams in the YRB. Site locations were selected using a multi-iteration ModEx approach. Sites span four sub-basins in the YRB and are distributed across multiple complementary efforts that each focus on time series (discussed here) or spatial variation (discussed in a separate presentation). The temporal component includes 6 sites distributed across stream orders and biomes from low order mountain settings to high order lowland rivers adjacent to agricultural and urban areas, coinciding with other agencies' gauging installations. The 6 sites have been visited every 1-2 weeks starting in April 2021 to collect *in-situ* measurements and water samples for standard measurements (e.g., organic C concentration, ion chemistry, carbonate/bicarbonate speciation) and less standard measurements (e.g., FTICR mass spectrometry), to provide model-relevant data. Initial analysis of the FTICR data indicates that many organic matter characteristics vary with catchment area. Specifically, both organic matter functional diversity, as it relates to biodegradability, and the potential for varied biogeochemical organic matter transformations increased with increasing catchment area. Starting in November 2021, preliminary deployments of automated dark-bottle incubation systems (autochambers) were initiated. These autochambers are designed to estimate the fraction of system respiration from sediments by measuring the difference between water column and ecosystem respiration rates in the river corridor. These are novel sensor systems, and the initial deployments are designed to generate time-series data and test/improve system function and reliability prior to larger-scale deployments. Data reduction and QA/QC has been developed and employed to generate sensor-based datasets. Lab analysis of samples is completed as samples are generated, and QA/QC is ongoing. These sensor- and sample-based time series will be used to drive and evaluate reaction networks in the dynamic basin-scale models used by the RCSFA.

The Influence of Wildfire Disturbance on River Corridor Hydrobiogeochemical Function

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BER Program: ESS
Project: PNNL River Corridor SFA (RCSFA)
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Project Abstract: *This element of the RCSFA aims to reveal the mechanisms by which wildfires influence biogeochemical cycling in river corridors from reaction to basin scale. Our objective is to improve model predictive capacity in watersheds impacted by fire disturbances, important for ascertaining the influence of fire on ecosystem structure and function*. Wildfires generate a spectrum of physical and chemical alterations to terrestrial vegetation (i.e., char and ash), which alter runoff materials entering inland waters; these altered materials and pathways can change aquatic ecosystem functions. Recent thermodynamic modeling work supports emerging theories that pyrogenic organic matter (PyOM) – a portion of these materials – is more bioavailable than traditionally accepted, supporting growing evidence that it may be an underappreciated driver of river corridor biogeochemistry. Most research on changes in char chemistry focuses on the continuum of combustion temperatures created in the laboratory and does not target shifts in burn severities seen in the landscape. Therefore, we designed and implemented an open-air burn table experiment to investigate how chemistry of vegetation-derived chars and their leachates changes with burn severity metrics. Initial experiment results showed organic phosphorus (P) was increasingly converted to calcium-associated inorganic P forms in chars with higher burn severity, while total percent carbon (C) and nitrogen (N) increased from parent feedstock to low severity burns, then subsequently decreased with increasing burn severity. We found higher severity burns had lower concentrations of dissolved C and N than lower severity burns, and shrubland feedstocks were more soluble than conifer feedstocks. These contrasting changes to organic matter (OM) and inorganic nutrient composition indicate that wildfires in different ecosystems may uniquely impact downstream riverine biogeochemical processes across common wildfire fuel types. Differences in OM chemistry at the landscape scale are also being examined through high resolution storm sampling across 5 western Oregon watersheds in the Holiday Farm Fire burn perimeter. We find that post-fire storms elevated the transport of surface materials to streams within the burn perimeter in which the quality of material delivered was controlled primarily by burn severity within the catchment. Additionally monthly changes in OM chemistry are being investigated in a semi-arid sub-watershed of the Yakima River Basin. We are modeling and monitoring in- and out-of-fire impacted stream reaches in the context of shifting C:N:P dynamics to assess the influence of fires on the relationships between C, N, and P cycling.

Hydrobiogeochemical Features and Function Across Basins

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Project: PNNL River Corridor SFA (RCSFA)
Project Website: https://www.pnnl.gov/projects/river-corridor

Project Abstract: *This element of the PNNL River Corridor SFA combines molecular data and numerical modeling to provide transferable principles that integrate organic matter (OM) chemistry and microbial gene expression.* We extend the RCSFA to the globe using crowdsourcing to further establish ESS as a global leader in open watershed science. We are leveraging WHONDRS data while shifting the sampling paradigm to efforts guided more directly by models, via deeper stakeholder engagement, and in partnership with other ESS investments and other agencies (e.g., USDA, NSF, DoD). For example, we are using AI models to guide new sampling locations (see ICON-ModEx presentation) and partnered with EXCHANGE and the University of Quebec to study OM chemistry from source to sea along the St. Lawrence River. We are also expanding to additional continents such as Africa and South America. From each of these sampling efforts, we also generate metagenomic and metatranscriptomic data with JGI. These data are being integrated into the Genome Resolved Open Watersheds database (GROWdb). GROWdb goes beyond the RCSFA and provides an open resource for global river corridor microbiomes. To date, 360 river microbiomes have been sampled across the globe and ongoing sampling aimed at filling in geographical gaps. Microbiomes from all sites were characterized using genome resolved metagenomics, enabling the reconstruction of thousands of unique microbial genomes and a corresponding catalog of over 2 million microbial genes, including sampling of 850 genes with known capacity to modulate carbon, nitrogen, sulfur, and hydrogen cycling in these watersheds. GROWdb has partnered with DOE KBase to make this resource publicly available and to enable integration of river-specific microbial processes into reactive transport models through genome-scale metabolic models, with 2,093 models built to date. Approximately a third of the samples have paired metatranscriptomes and metabolomes, distinguishing active from latent microbial processes and providing additional constraints for modeling efforts.

Mechanisms Governing Spatial Variability in River Corridor Hydrobiogeochemistry

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Project: PNNL River Corridor SFA (RCSFA)
Project Website: https://www.pnnl.gov/projects/river-corridor

Project Abstract: *This element of the PNNL River Corridor SFA seeks to understand spatial variability in hydrobiogeochemistry across the Yakima River Basin (YRB).* To represent processes governing river corridor hydrobiogeochemistry in models, we need to understand hydrobiogeochemistry across broad environmental gradients that include natural (e.g., fire) and anthropogenic (e.g., urban) disturbances. To help fill this need we are studying spatial variation in river corridor chemistry, microbiology, and aerobic respiration across 47 sites in the YRB. Sites were selected using an iterative ModEx approach. Integrated teams selected model-relevant variables for both standard (e.g., dissolved organic C concentration, major ion chemistry) and less standard measurements (e.g., organic matter chemistry via FTICR). Numerical simulations were coupled with AI methods to identify system features most strongly associated with predicted variation in river corridor hydrobiogeochemistry. These key features were used to cluster YRB rivers into classes. Field sites were selected across all classes while accounting for logistical constraints of field work. Resulting sites were distributed across stream orders, biomes, and land cover/land use from low order mountain settings to high order lowlands adjacent to urban and agricultural settings. One key measurement was water column respiration, assayed using *in situ* dark bottle incubations. We found that water column respiration increased with stream order. This is counter to previous work showing that CO_2 (a product of respiration) evasion from streams decreases with increasing stream order. This also implies that the fraction of ecosystem respiration from sediments may decrease with stream order. If so, that would reject current model predictions; a field campaign in summer 2022 will test this hypothesis and outcomes will guide model refinements and updated model predictions. Further, our work both rejects and supports the River Continuum Concept (RCC). The RCC predicts that organic matter (OM) chemistry will vary down the stream network. Consistent with the RCC, OM diversity increased down the network. In contrast, processes governing OM chemistry were similar at the top and bottom of the network, but distinct in the middle. These results point to a need to revise some of the conceptual and mechanistic foundations of river corridor hydrobiogeochemistry.

Improving Knowledge and Predictions of Hyporheic Zone Respiration via Continental-Scale Iterative ICON-ModEx Science

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Project: PNNL River Corridor SFA (RCSFA)
Project Website: https://www.pnnl.gov/projects/river-corridor, https://whondrs.pnnl.gov, https://www.pnnl.gov/projects/WHONDRS/icon-modex, https://icon-science.pnnl.gov

Project Abstract: *This element of the PNNL River Corridor SFA is focused on improving predictive understanding of hyporheic respiration.* The Earth's biogeochemical and water cycles are tied closely to river corridors and stream respiration. Microbes in hyporheic sediments have a wide range of influence over river corridor biogeochemistry; hyporheic zones contribute from 4 to 96% of stream respiration. This project addresses the uncertainty of predicting this variation. We are combining public data, artificial intelligence (AI) and mechanistic modeling, ICON principles, and model-experiment (ModEx) iteration via crowdsourced sampling across the contiguous United States (ConUS). ICON principles, facilitated via the ICON Science Cooperative, are used by Integrating AI modeling with biogeochemistry, Coordinating protocols to be consistent with previous efforts, Openly sharing ideas and data, and Networking with stakeholders to increase mutual benefit of outcomes. The project started with data from the Worldwide Hydrobiogeochemical Observation Network for Dynamic Rivers (WHONDRS) to develop a suite of AI models to predict respiration rates at unsampled locations across the ConUS. Due to limited data, the model has biased predictions at high respiration rates. The project is working to improve the model and determine which variables drive hyporheic zone respiration rates. To address inaccuracies in model predictions, we guide volunteers to high priority locations across the ConUS for new sample collection. Both open stakeholder engagement and model needs will determine sample collection and data generation. Results will be fed back into the model to make new predictions and guide additional sampling, with the aim of multiple ModEx iterations. Once the respiration model is refined, it will be incorporated into basin-scale mechanistic hydro-biogeochemistry modeling, which will quantify how basin-scale fluxes of carbon and nutrients are impacted by variation in hyporheic respiration.

SLAC Floodplain Hydro-Biogeochemistry SFA: Spatiotemporal Response of Soil-Gravel Bed Connectivity to Hydrological Transitions in an Intermountain Floodplain Aquifer

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Project: SLAC Floodplain Hydro-Biogeochemistry SFA
Project Website: https://sites.slac.stanford.edu/bargargroup/news

Project Abstract: Riparian environments in the Intermountain West are often characterized by extensive interfaces between basal gravel/cobble alluviums and overlying fine-grained soils, which exhibit sharp redox and solute concentration gradients that mediate subsurface water quality. The biogeochemical function of these interfaces results from a tight coupling between hydrological and biogeochemical processes. In particular, the hydraulic connectivity between the gravel bed and the soil dictates the direction and intensity of solute exchanges, and consequently the capacity of the floodplain system to act as a sink or as a source for redox-sensitive nutrients or contaminants (*e.g.* Fe, C). Yet, the spatial evolution of this connectivity and its response to hydrological shifts remain poorly understood.

Our combined field and numerical modeling work on our field site of Slate River, CO, highlights the ways in which the gravel bed controls floodplain hydrology. Due to its large volume and hydraulic conductivity, the gravel bed acts as a preferential flowpath for regional subsurface flow in the down-valley direction, and shows a strong connection with surface water with fast response to hydrological shifts. In contrast, the overlying riparian soils correspond to a hydraulic transition zone between the gravel bed and the surface water, that accommodates smaller-scale hydro-geomorphological features such as the presence of a beaver pond. During snowmelt, rapidly rising water tables in the gravel bed impede downwards surface water infiltration and increase water residence times in the soil. During baseflow, declining water tables in the gravel bed drive more surface water into the soil and through the soil-gravel bed interface. Our work also indicates that the mostly downward flow direction at the soil-gravel bed interface may occasionally reverse, for instance in the return flow areas downstream of beaver dams, or in the distal areas from the stream where evapotranspiration becomes dominant over lateral surface water recharge. These results highlight how hydrologic dynamics and hydraulic connectivity help mediate intermountain floodplain function.

SLAC Floodplain Hydro-Biogeochemistry SFA: Colloid Dynamics at Floodplain Soil-Gravel Bed Interfaces

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Project: DOE SLAC-SFA Program (lead: Kristin Boye)
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Project Abstract: Subsurface interfaces are ubiquitous in floodplain environments and sustain a multitude of biogeochemical processes, including the formation and release of reactive, mobile colloids. Colloids are known vectors of micronutrient, contaminant, and organic matter transport and are suspected to be important export agents from floodplains to stream water. However, few studies have documented the impact of seasonally-variable field hydrological and geochemical dynamics on redox-active colloid occurrence, and transport in riparian floodplains.

We used a combination of cascade filtering, advanced analyses of field samples, lab-based column experiments, and reactive transport modelling (RTM) to characterize the fate of Fe-rich colloids at our floodplain field site of Slate River, CO. Cascade filtering revealed the presence of Fe-rich colloids in the riparian anoxic soil water, whose abundance and composition vary with season and depth, suggesting a strong link to hydrological and biogeochemical dynamics. Cryo-EM and TEM-EDS imaging showed mono-dispersed and nano-assemblages of spherical colloids in the 10-50 nm range containing Fe, O, Si, C, and Ca. Mössbauer spectroscopy indicated a poorly crystalline ferrihydrite-like phase, coated with organic matter and Si. Fe-EXAFS further verified ferrihydrite and Fe(II)- and Fe(III)-organic matter interactions. We therefore conclude the colloids are primarily composed of nanosized ferrihydrite spheres that are stabilized by organic matter, Si, and bridging cations (e.g., Ca). The fact that these Fe(III)-rich colloids existed in primarily anoxic zones is striking. We postulate that the Si-organic matter coating provides a primary protective layer against reduction, but its efficiency depends on the biogeochemical and hydrological conditions. In spring, porewater flow velocity was low in the anoxic soil, due to rising water table, and a higher abundance of Fe(II)-rich colloids was observed. We hypothesize that longer residence times coupled with high organic matter levels, contribute to the formation of the reduced, nanosized colloids. At baseflow, in summer and autumn, increased downward infiltration appears to flush the colloids into to the gravel bed, where relatively high (1.5 m/day) flow velocities may transport them to the river. Furthermore, findings from our column experiments coupled with reactive transport simulations suggest that organic matter-bearing colloids may substantially alter the biogeochemical functioning of the gravel bed itself.

SLAC Floodplain Hydro-Biogeochemistry SFA: Hydrological and microbiome dynamics drive shifts in subsurface geochemistry and oxic-anoxic interfaces in floodplain soils

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Project: SLAC Floodplain Hydro-Biogeochemistry SFA
Project Website: https://sites.slac.stanford.edu/bargargroup/news

Project Abstract: Subsurface microbial communities in floodplain soils drive major biogeochemical cycles (e.g., C, N, S) and control the fate and transport of many metals and contaminants (e.g., Fe, Mn, Zn). Each year floodplains experience seasonal rise and decline of the water table that determines nutrient and other inputs to the subsurface, as well as the oxygen penetration depth. Within the soil column, the boundary depth between oxic and anoxic conditions is therefore controlled largely by floodplain hydrology. Snowmelt-induced flooding and other precipitation further contribute to shifts in the depth of this oxic-anoxic interface. Thus, it is critical to define connections between seasonal hydrology and changes in microbial community composition (and function), as these are not yet well understood.

In our study site along the Slate River, CO, we observe two types of interfaces, namely: (1) an oxic-anoxic interface within the fine-grained layer, as well as (2) a deeper physical interface where soils/sediments shift to a coarse cobble layer. This cobble layer is more directly connected to the river, with oxygenated groundwater moving through it, thus forming a secondary oxic-anoxic interface deeper in the soil column. Using these two interfaces as a guide, we investigated microbial community composition across multiple depths (~10-30 cm resolution) and time points from 2018-2021 at two Slate River floodplain sites. This spatiotemporal analysis consistently revealed phylogenetically- and metabolically-diverse populations of bacteria and archaea, including methanogens and methanotrophs, sulfur-oxidizing and -reducing taxa, ammonia-oxidizing archaea, and iron-cycling bacteria. These communities showed a striking depth distribution across oxic-anoxic boundaries; for example, within the *Archaea*, ammonia-oxidizing *Thaumarchaeota* were abundant in shallow oxic soils, whereas methanogens and *Bathyarchaeota* were found exclusively in deeper anoxic soils. We also investigated the impact of hydrologic perturbations on subsurface microbial communities and geochemistry, through field inundation experiments as well as the coincidental construction of a beaver dam at one site in 2019. The resultant flooding caused microbial community shifts that are reflected in observed geochemistry, as well as modeled oxygen penetration depth. Further analyses, including genome-resolved metagenomics and metatranscriptomics, will be employed to examine floodplain microbiome dynamics at an even finer scale and connect both hydrology and geochemistry to specific biogeochemical processes.

Title: The AmeriFlux Rapid Response System

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BER Program: ESS

Project: AmeriFlux Management Project

Project Website: http://ameriflux.lbl.gov/

Project Abstract: Beginning in 2014, the AmeriFlux Management Project has pioneered a program that allows scientists to rapidly initiate ecosystem flux measurements, to take advantage of special research opportunities. Specifically, we maintain and make available loaner flux systems (Rapid Response Systems; RRS) suitable for quick deployment to help scientists capture valuable research opportunities that arise unexpectedly or have limited measurement windows. The RRS is a stand-alone instrument package with a full complement of flux (carbon, water, and energy), meteorological (relative humidity, air temperature, barometric pressure), and radiation sensors (4-component net radiometer, and photosynthetically active radiation). Power and tower infrastructure are not standard components of the RRS and historically have been provided by the RRS requester. Since 2014, AMP has built five RRS and each was immediately in demand. They have been deployed for:

- Ecosystem response to wildfire in northern New Mexico (PI: Marcy Litvak, Sept. 2014–March 2018);
- Plant species composition change in coastal wetlands, Kennedy Space Center, Florida (PI: Ross Hinkle, March 2017–TBD);
- Large-scale irrigation experiment in rice fields, Arkansas (PI: Ben Runkle, May 2019–Nov. 2020);
- Pinyon-juniper recovery following severe drought in southern Utah (PI: Dave Bowling, June 2019–May 2022);
- Post-fire recovery research in a ponderosa pine forest in Oregon (PI: Chris Still, October 2021- September 2024).

The RRS program is successful and we are anticipating the deployment of several RRS in support of synergetic activities across DOE programs: (1) A deployment in August 2022 in support of the SAIL Campaign (Sept. 2021 through June 2023) in the East River Watershed of the Rocky Mountains (https://sail.lbl.gov/), where they would be used to improve representation of processes affecting modeling of climate and mountainous hydrology; (2) A deployment along with an upcoming multi-year ARM Mobile Facility campaign in the Southeastern United States in 2023 for five years (SEUS;

https://arm.gov/capabilities/observatories/amf/locations/seus). This campaign aims to enhance process understanding and model representations of aerosol, cloud, and land-atmosphere interactions.

To support the growing interest in using the eddy covariance technique in urban environments, the AmeriFlux Management Project has built two additional RRS. These systems (CO_2, H_2O, CH_4, and energy) are similar to previously deployed RRS but are dedicated to deployment in urban environment. These observation packages could support the new BER initiative on Urban Integrated Field Laboratories (Urban IFLs) that will build integrated models and tools to improve our understanding of the links between the natural and human components of the climate system.

Title: **AmeriFlux Community Initiatives**

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Project: DOE Lab-led project: AmeriFlux Management Project (LBNL)

Project Website: https://ameriflux.lbl.gov/

Project Abstract: Community collaboration initiatives are at the core of how AMP enables the community to do transformative research. Examples of such initiatives include focal theme years, workshops, webinar and seminar series, annual community meetings and town halls at conferences. Here we describe a subset of recent and planned initiatives focused on supporting the broader AmeriFlux community.

As part of our community collaboration initiatives, we host theme years of focal interest. We recently launched the Year of Water Fluxes as our next theme year for community action. There are many science opportunities to study water fluxes in AmeriFlux. This theme year will support more water cycle measurements, enhance data quality, and build strong collaborations to work on the various aspects of water and fluxes. Initial activities included an Evapotranspiration workshop focused on measurements of water fluxes between ecosystems and the atmosphere (Nov 2-4th) (https://ameriflux.lbl.gov/community/ameriflux-meetings-workshops/) and a water focused AmeriFlux Annual Meeting. More activities and opportunities for engagement with the community are planned over the coming year.

This year also saw the launch of a new LBL and community-led project focused on FLUXNET, the global network of eddy-covariance research networks. The central goals of the NSF funded FLUXNET coordination project are to provide novel training and exchange opportunities, develop strong international collaborations, and build tools and protocols that ensure continued collaboration and growth. To do so, the FLUXNET coordination project will develop both data-focused processing protocols and pipelines, and people-focused education and exchange opportunities. Through the FLUXNET coordination project, we will use creative and transformative approaches to international collaboration and networked science, to build the next generation of FLUXNET to be a self-sustaining flagship of networked global scientific cooperation.

Title: **Diversity, Equity and Inclusion Initiatives for a Coalition of the Willing**

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Project: DOE Lab-led project: AmeriFlux Management Project (LBNL)

Project Website: https://ameriflux.lbl.gov/

Project Abstract: The AmeriFlux Network is a community of providers and users of eddy covariance flux data. The level of commitment and engagement in the community encompasses a wide spectrum; from mere mailing-list membership, to participation in community events, to sharing best practices and data, to direct operational support for some long-term sites. Members work at institutions from various countries, with various funding levels, and institutional standards around physical and psychological safety. This heterogeneous membership poses particular challenges for Diversity, Equity, and Inclusion (DEI) initiatives.

Driven by member interest, we formed the AmeriFlux DEI committee to understand and address the needs of our diverse community. In the past year, we have identified DEI blind spots via community surveys and panels, and created corresponding resources (e.g., a handbook for safe and inclusive fieldwork). We hope to continue engaging with our community to improve open and inclusive science across AmeriFlux and beyond.

Title: Making AmeriFlux Data More Open and Cite-able

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BER Program: ESS

Project: DOE Lab-led project: AmeriFlux Management Project (LBNL)

Project Website: https://ameriflux.lbl.gov/

Project Abstract: AmeriFlux has added a new CC-BY-4.0 data usage license (Creative Commons by Attribution 4.0 International; https://creativecommons.org/licenses/by/4.0/) and so far 374 of the 567 AmeriFlux sites have chosen this license. This new AmeriFlux CC-BY-4 data license makes AmeriFlux data more compatible with other flux networks (e.g. ICOS, OzFlux, and NEON) and FAIR (Findable, Accessible, Interoperable, and Reusable).

It is also a first step toward making the data easier to use and cite. A remaining challenge has been citing the AmeriFlux data in scholarly works where data from a large number of sites are used. A Community of Practice has been working for the last year to develop an approach that will allow 100's of citations to be included as references in a paper through the use of a mechanism referred to as a “reliquary.” The AmeriFlux data case is one of the leading use cases in the development of the solution. The Community of Practice is composed of volunteers from across the Earth sciences community including publishers, data repository representatives, leaders of large-scale projects, AGU data management leaders, UN Climate Assessment groups, citation indexers, DataCite, RDA, and government agencies. To learn more about the work of the Community of Practice and to join us if you are interested, visit https://data.agu.org/DataCitationCoP/.

Title: **Multiscale Data Synthesis and Analysis for Understanding Coastal Ecosystems**

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Project: COMPASS-FME
Project Website: https://compass.pnnl.gov/fme

Project Abstract: This multipronged data synthesis effort involved five key areas clearly and traceably linked with the main COMPASS-FME hypotheses and/or goals, and highly relevant for the project's modeling and/or experimental goals. These areas are to (i) assemble and synthesize disparate coastal datasets relevant to the project; (ii) use a meta-analysis to understand how top-of-column root- and/or microbe-generated greenhouse gas fluxes are affected by changes in water availability, experimental length, and ecosystem type; (iii) examine how inundation changes alter vegetation dynamics and lead to the formation of 'ghost forests' worldwide, and the mechanisms driving these changes; (iv) use machine learning to probe how estuarine and lacustrine water biogeochemistry and quality vary through time and space, and the effects of press and pulse disturbances; and (v) understand the degree to which coastal marsh plant production is driven by growing season phenology, tidal flooding, and species-specific effects. Finally (vi), a 'functional zonation' task focusing on spatial synthesis and inference is being used to scale results and models within COMPASS-FME as well as to the larger-scale companion project COMPASS-GLM.

We summarize progress in these areas, including initial results, the manuscripts submitted and published to date, and how this work links with other project MODEX efforts. Key results include the construction of a meta-analysis statistical pipeline for (ii), and ingestion of over 100 studies reporting soil water manipulation experiments; a completed literature review in (iii) that provides the foundation for a testable framework regarding ghost forest formation under changing inundation levels; extensive dataset assembly and analysis in (iv) working to identify linkages between water quality, ephemeral ecosystem control points, and disturbances; and an ongoing belowground traits meta-analysis (v) focusing on how these factors control coastal marsh productivity in the Chesapeake Bay (CB) region. Finally, the functional zonation team has assembled and co-registered spatial datasets across the CB and Lake Erie regions (vi), constructed maps of the functional zones in which the project's synoptic sites sit, and finalized regression models predicting peak plant productivity.

Title: **Multiscale Observations and Modeling for Improved Prediction of Coastal Wetland Processes**

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BER Program: ESS
Project: COMPASS-FME
Project Website: https://compass.pnnl.gov/fme

Project Abstract: COMPASS-FME has established field sites for intensive synoptic studies in two distinct geographies: in brackish marsh systems of the Chesapeake Bay, and in freshwater wetlands of the Western Lake Erie Basin. Within each region, three sites were selected to establish transects that span elevation gradients consisting of coastal upland forests, forest-wetland transitions, wetlands, and nearshore open waters. The sites also lie along regional gradients in salinity in the case of Chesapeake Bay and gradients in nutrient loading and geomorphology in both regions. Measurements that are being made now and are planned for the coming season include observations of subsurface and surface biogeochemical, plant physiological, hydrological, and geophysical processes. Modelers and observationalists are working together to define multi-scale measurements and simulations to elucidate processes at each site. Modeling is being conducted at point, column, and transect scales using a hierarchy of process-resolving models. Simulations of biogeochemistry at the scale of the soil pore space are capturing microbial dynamics, redox reaction networks, organic matter decomposition, and gas flux. Simulations in single vegetation/sediment/soil columns include those pore-scale dynamics, and introduce variability along vertical gradients in temperature, moisture, oxygen concentration, salinity, and organic matter composition. Two-dimensional transect simulations integrate pore-scale and vertical dynamics along the horizontal transition from wetland to upland conditions, including the effects of inundation from the wetland side and freshwater flooding from the upland side. Here we present results from simulations at each of the three scales (pore, column, transect), based on preliminary observations from COMPASS-FME synoptic sites. These results have helped to refine COMPASS-FME field activities, prioritizing measurements to be gathered in the upcoming field season. For example, we are prioritizing physical characterization of soils, quantifying interactions between iron and sulfur cycles, and extending measurements of plant physiology across all the synoptic sites.

Title: The Exploration of Coastal Hydro-biogeochemistry Across a Network of Gradients and Experiments Consortium (EXCHANGE)

Allison N. Myers-Pigg[1*], Allison Lewis[3], Peter Regier[1], Kaizad Patel[1], Khadijah Homoka[1], Opal Otenburg[1], Stephanie Pennington[1], Nicholas Ward[1], Ken Kemner[4], Vanessa Bailey[1], EXCHANGE Consortium

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Project Lead Principal Investigator (PI): Vanessa Bailey
BER Program: ESS
Project: COMPASS-FME
Project Website: https://compass.pnnl.gov/fme; https://compass.pnnl.gov/fme/EXCHANGE

Project Abstract: The EXCHANGE Consortium aims to improve understanding of how the two-way exchange of water between estuaries or large lake lacustuaries and the terrestrial landscape influence the state and function of ecosystems across diverse coastal interfaces. Our overarching goal is to develop a community-driven, regionally distributed sampling network to examine how spatial variations lead to ecosystem control points at the coastal terrestrial-aquatic interface (TAI). We are using a combination of bulk measurements, molecular level analyses, and laboratory experiments on soil, sediment, and water samples collected across transverse gradients (from upland to estuarine waters – the coastal terrestrial-aquatic interface) at geographically distributed sites around two major coastal regions—the Mid-Atlantic and the Great Lakes. These geographically distributed measurements and experiments will enable us to elucidate how organic matter (OM) cycling dynamics vary between saline and freshwater coastal TAIs, respectively. We are studying the spatial variability in coastal ecosystem dynamics through a series of targeted campaigns. Campaigns developed via workshops with regional partners follow ICON-FAIR principles from conception to data analysis and publication. The first EXCHANGE campaign (EC1) focuses on baseline understanding of the chemical forms and distribution of carbon and nutrients across research sites in both regions. During the Fall of 2021, participants in EC1 collected samples from 52 coastal TAIs using standardized sampling kits. Experiments were performed on samples from a subset of sites to evaluate the response of soil and sediment greenhouse gas production to inundation. Spatial variation across regions was apparent across multiple data types, with variability in surface water chemistry (e.g. dissolved organic carbon, nitrate/nitrite) greater in the Mid-Atlantic compared to the Great Lakes. Spatial variations in terrestrial and aquatic biogeochemical properties and processes studied as a part of EXCHANGE are the product of a range of different environmental conditions, geomorphic settings, and inundation history. For example, total carbon in transition zone soils was lower in soils with visually observed iron oxidation. The data produced by EXCHANGE increase our understanding of how OM processing and transport is coupled to depth and duration of soil saturation and the abundance of redox-sensitive elements, which is essential to the parameterization of reactive transport modeling across spatial scales.

Title: **The Terrestrial Ecosystem Manipulation to Probe the Effects of Storm Treatments Experiment**

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BER Program: ESS
Project: COMPASS-FME
Project Website: https://compass.pnnl.gov/fme

Project Abstract: Coastal upland forests are facing widespread mortality as sea-level rise accelerates and precipitation and storm regimes change. The loss of coastal forests has significant implications for the coastal carbon cycle; yet, predicting the likelihood of mortality is difficult due to our limited understanding of disturbance impacts on coastal forests. The manipulative, ecosystem-scale Terrestrial Ecosystem Manipulation to Probe the Effects of Storm Treatments (TEMPEST) experiment is designed to address the potential for extreme freshwater and seawater disturbance events to alter tree function, species composition, and ecosystem processes in a deciduous coastal forest in Maryland, USA. The experiment uses a large-unit (2,000 m^2), un-replicated experimental design, with three 50-m x 40-m plots serving as control, freshwater, and seawater treatments. Transient saturation (5 hours) of the entire soil rooting zone (0-30 cm) across a 2,000 m^2 coastal forest is attained by delivering 300 m^3 of water through a spatially distributed irrigation network at a rate just above the soil infiltration rate. Our water delivery approach also produces extensive, low-level (≤ 8 cm above ground) inundation and elevates the water table, which is typically ~5 m below ground. A TEMPEST simulation approximates a 15-cm rainfall and based on historic records, is of comparable intensity to a 10-year storm for the area. Treatment application frequency will increase over a decade to quantify tipping points where plant and microbial communities and biogeochemical cycles begin to change rapidly. Pre-treatment data collection began in 2019 and the first full simulation is scheduled for June 2022. This experimental framework provides us with an unparalleled opportunity to control disturbance frequency and intensity and disentangle the effects of saturation and salinity under in-situ conditions and at an ecosystem-scale.

Title: **Simulations of Duke and Oak Ridge FACE Experiments with ELM-FATES-CNP**

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BER Program: ESS

Project: Free Air CO_2 Enrichment Model Data Synthesis (FACE-MDS) (DOE Lab-led project)

Project Website: https://facedata.ornl.gov/facemds

Project Abstract: The response of temperate forests to elevated atmospheric CO_2 (eCO2) can be constrained by the short-term dynamics of nitrogen (N) availability, which can interact with longer-term demographic processes. Understanding the interactions of N availability with forest growth processes as N is locked away in plant biomass and soils and then released as plants die and soils decay is necessary to develop predictive understanding of forest ecosystem responses to eCO2 at climate-change relevant timescales (i.e. decades). Long-term Free Air CO_2 Enrichment (FACE) experiments, such as Duke and Oak Ridge, ran for a single decade, providing information on eCO2, N, and demographic process interactions. We use these data to constrain simulations by the Functionally Assembled Terrestrial Ecosystem Simulator (FATES), a model with tree-size and time since disturbance resolution, embedded within the ELM land surface and terrestrial biosphere model. A model with a representation of size structure allows us to evaluate how size-structure and demographic processes may have influenced results at the Duke and ORNL FACE experiments, asking the question: How have demographic processes shaped the responses to eCO2 observed at long-term FACE experiments? Recent developments to bring nutrient cycling into ELM-FATES (ELM-FATES-CNP) now provide the N and other nutrient-related constraints within the model to simulate and evaluate eCO2, N, and demographic process interactions. In this spark presentation, we apply ELM-FATES-CNP to simulating the Duke and Oak Ridge FACE experiments. We use a C-only version of the model alongside two soil nutrient cycling hypotheses or conceptualizations that currently exist in ELM—relative demand and equilibrium chemistry approximation—modified to represent a dynamic allocation scheme that is more consistent with the data. Here we show that ELM-FATES-CNP can reproduce baseline, ambient treatment values of key ecosystem variables. eCO2 responses can depend on N dynamics but the magnitude of the N constraint is highly dependent on the V_{max} parameter values for N uptake. We also begin to investigate stand structure dynamics showing that the simulation

of a plantation forest and forest-structure more broadly is highly dependent on the specific assumptions made regarding crown, leaf, and sapwood allometry.

Linking Molecular Characterization with Continuum Reactive Transport Modeling

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BER Program: ESS

Project: **IDEAS-Watersheds**

Project Website: https://ideas-watersheds.github.io/

Project Abstract:

The IDEAS-Watersheds focuses on developing flexible modeling capabilities and workflows through contributions to a community-driven software ecosystem that advance hydrobiogeochemical research in watersheds and river corridors.These contributions are in turn made available to the broader community. For example, we have developed a modeling pipeline from molecular characteristics, such as organic carbon speciation, to biogeochemical models and to continuum reactive transport models. Leveraging the DOE's KBase modeling platform, we have prototyped the two key steps of this pipeline as KBase Apps using the KBase Software Development Kit: one for translating chemical compositions from FTICR-MS into biogeochemical reaction models, and one that takes those reaction models and sets them up as 1-D reactive transport models with PFLOTRAN. After testing those new reaction networks and kinetics, which were informed by the organic carbon speciation, in PFLOTRAN in batch and column configurations, we incorporated those reaction models in ATS-PFLOTRAN for coupled hydrologic and biogeochemical modeling at the American River watershed. We used this coupled watershed model to investigate water, energy, and solute fluxes across the river-groundwater interface. The biogeochemical hot spots and hot moments within the river corridors are found to be strongly influenced by riverbed properties and flow conditions, and hence, influenced by variations in land use, hydrogeology, climate, and disturbances. This pipeline can be extended to allow the incorporation of other omics datasets (such as metatranscripts, metaproteomics and metabolomics) when they become available. We have shared our KBase narrative examples with the broader community to enable leveraging the pipeline in hydrobiogeochemical studies on other watersheds and river corridors. Finally, we note that the

ATS-PFLOTRAN coupled watershed model is an example of interoperable model development, where generic interfaces such as the Alquimia biogeochemistry interface library, extend the capabilities available from single codes in the software ecosystem by bringing their complementary capabilities together.

Progress Toward Scale-consistent Watershed Reactive Transport Models

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Project: IDEAS-Watersheds

Project Website: https://ideas-watersheds.github.io/

Project Abstract:

Most watershed-scale models focus on hydrological processes with limited capacity to represent the complex biogeochemical processes that control the efflux of greenhouse gases and the waterborne exports of carbon, nutrients, and trace metals. The IDEAS-Watersheds project in partnership with multiple watershed Science Focus Areas has been addressing that capability gap by extending parallel spatially resolved integrated surface/subsurface hydrology models to include reactive transport. The new capability addresses the central modeling challenges: coupling reactive transport across the surface and subsurface spatial domains, and tractably representing the effects of fine-scale biogeochemical phenomena without resorting to ad hoc upscaling. Those advances were enabled by software capabilities advanced by the IDEAS project including new approaches for multiphysics model coupling, mesh infrastructure that allows for multiple coupled meshes, and the application programming interface Alquimia, which provides hydrology codes access to widely used biogeochemical codes.

The Advanced Terrestrial Simulator (ATS) has been extended to couple multicomponent reactive transport across the surface water and subsurface domains (Molins et al., 2022). The integrated model has been used to investigate the response of the Copper Creek subwatershed in the East River, Colorado, Watershed over a ten-year period (Xu et al., 2022). Current modeling efforts focus on the Lower Triangle region to understand the processes affecting nitrogen exports with consideration of spatially-distributed watershed properties.

We have also developed a novel multiscale modeling approach (Jan et al. 2021) to represent the watershed-scale effects of biogeochemical transformations within small-scale biogeochemical

hotspots. We have implemented this model in ATS, used it to estimate model parameters from stream tracer tests (Rathore et al. 2021), demonstrated it on East Fork Poplar Creek Watershed and the Portage River Basin (Jan et al. 2021), and developed the workflow to build watershed-scale models from online data sources. We plan to extend the model-building workflow to improve estimates of hyporheic exchange flows using classification of hydrogeomorphic features.

These are first-of-a-kind capabilities that consider surface and subsurface reactive transport as an integrated multiscale system, thus improving representations of dynamic surface/groundwater exchanges, allowing for different reaction systems in the surface and subsurface, and avoiding *ad hoc* upscaling. We have plans to include additional watershed processes and integrate these new capabilities to provide a scale-consistent watershed reactive transport modeling tool that can be used to advance understanding of watershed hydro-biogeochemical function.

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Title: **National datasets and workflows for integrated hydrologic modeling across the US**

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BER Program: ESS

Project: IDEAS-watersheds

Project Website: https://ideas-watersheds.github.io/

Project Abstract:

The ParFlow-CONUS simulation platform has been in ongoing development for a decade and spans input data, several decades' worth of simulations, and comprehensive analysis tools to make the input and output data publicly available. This work has resulted in many publications that have advanced both technical capabilities for large-scale simulation, as well as scientific understanding of continental-scale hydrologic interactions including how transpiration and groundwater are linked, how the US' legacy of groundwater pumping has impacted the rest of the hydrologic cycle and how climate change may impact our groundwater resources both regionally and locally). Work is now focused on version 2 of the model (CONUS2.0) which expands from version 1 to cover the entire drainage area of the contiguous US. Over the last year we have published several publications that detail new national dataset development (Zhang et al 2021; Steyaert et al 2022), model intercomparison with the US National Water Model (Tijerina et al 2021), and a detailed evaluation of long-term version 1.0 simulations (O'Neill et al 2021).

Key to the successes of the ParFlow-CONUS platform are interoperable workflows that facilitate data and model development. While the static inputs to the model are small, forcing datasets for CONUS2.0 are much larger (~50TB in size) and the simulation outputs are expected to be almost 1PB. These large datasets have not only taken years to develop but are too large for traditional analysis approaches, and required our team to develop custom reproducible workflows in tandem with the dataset creation. To manage these large data sets and ensure the community can access them in practical ways, we are leveraging a dedicated datacenter (the Princeton Hydrologic Data Center, or PHDC) was constructed as a platform to store and serve these community resources.

In addition, our team has built subsetting workflows which have been used to construct regional models of the Upper Colorado (e.g. Tran et al 2022) and the Delaware-Susquehanna basins and will be available for the ESS community to use in their work.

This presentation will highlight the data-workflow-integration for high resolution continental- and regional-scale community model development and recent CONUS 2 accomplishments. National-scale model input datasets combine multiple sources and involve rigorous testing over both the entire CONUS 2 domain and subsets of it. The development of these data and how they improve the CONUS 2 simulation results will be discussed.

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Topography Drives Variability in Circumpolar Permafrost Thaw Pond Expansion

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One of the most conspicuous signals of climate change in high-latitude tundra is the expansion of thermokarst pools. These small but abundant water features form rapidly in depressions caused by the melting of ice wedges (*i.e.*, meter-scale bodies of ice embedded within the top of the permafrost). Pool expansion not only signals permafrost degradation, but strongly impacts subsequent thaw rates through a series of complex positive and negative feedbacks which play out over timescales of decades, the net effect of which may accelerate carbon release from the underlying sediments. Despite the importance of thermokarst pool expansion to assessments of contemporary permafrost thaw, historical observations are limited in spatial and temporal frequency. Here we present the most geographically extensive and temporally dense measurements yet compiled of recent pool expansion, in which changes to pool area from 2008—2020 were quantified through satellite-imagery analysis at twenty-seven landscapes dispersed throughout the circumpolar tundra. The results revealed instances of rapid thermokarst pool expansion at 44% of survey areas and in temperature settings that ranged from very cold to mild. The sites that experienced the greatest net change tended to be those with the greatest topographic relief (tens of meters of variation within an area of eight square kilometers). This pan-Arctic relationship was associated with an enhanced vulnerability of ice wedges near hilltops, as within most sites, the fastest growing pools were found on convex points on the land surface. These findings indicate the necessity of including topographic controls in global projections of permafrost thaw.

Spatial Patterns of Snow Distribution in the Sub-Arctic

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The spatial distribution of snow plays a vital role in sub-Arctic and Arctic climate, hydrology, and ecology due to its fundamental influence on the water balance, thermal regimes, vegetation, and carbon flux. However, the spatial distribution of snow is not well understood, and therefore, it is not well modeled, which can lead to substantial uncertainties in snow cover representations. To capture key hydro-ecological controls on snow spatial distribution, we carried out intensive field studies over multiple years for two small (2017-2019, ~2.5 km^2) sub-Arctic study sites located on the Seward Peninsula of Alaska. Using an intensive suite of field observations (>22,000 data points), we developed simple models of spatial distribution of snow water equivalent (SWE) using factors such as topographic characteristics, vegetation characteristics based on greenness (normalized different vegetation index, NDVI), and a simple metric for approximating winds. The most successful model was the random forest using both study sites and all years, which was able to accurately capture the complexity and variability of snow characteristics across the sites. Approximately 86% of the SWE distribution could be accounted for, on average, by the random forest model at the study sites. Factors that impacted year-to-year snow distribution included NDVI, elevation, and a metric to represent coarse microtopography (topographic position index, or TPI), while slope, wind, and fine microtopography factors were less important. The models were used to predict SWE at the locations through the study area and for all years. The characterization of the SWE spatial distribution patterns will be used to validate and improve snow distribution modelling in the Department of Energy's earth system model, and for improved understanding of hydrology, topography, and vegetation dynamics in the sub-Arctic and Arctic regions of the globe.

Dynamic Soil Columns Simulate Arctic Redox Biogeochemistry

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Arctic soil represents a large reservoir of organic carbon that is vulnerable to decomposition and release as carbon dioxide (CO_2) and methane (CH_4). Thawing permafrost landscapes are especially sensitive, with thermokarst formation dramatically changing Arctic hydrology and altering soil temperature regimes, oxygen availability, and biogeochemical redox cycling. There is limited understanding of how rapid redox transitions in Arctic soils will impact the magnitude and timing of CO_2 and CH_4 release. As ecosystem scale models advance to incorporate process-based soil redox biogeochemistry, improved mechanistic understanding of the links between hydrology, redox conditions, and microbial organic carbon decomposition will be required. This study identified shifts in Arctic soil microbial metabolisms due to changing oxygen availability during soil saturation and drainage. Dynamic soil column experiments were used to change the water level in soil and permafrost collected from an inundated thermokarst channel and the adjacent upland tundra near Council, Alaska. Soil columns (50 cm length, 7.5 cm diameter) were instrumented to continuously measure volumetric water content and oxygen concentrations and were operated at field-relevant temperatures and water contents. Discrete porewater samples were taken from MicroRhizon samplers and measured for ferrous and total iron, pH, dissolved organic carbon, and major cations, anions, and organic acids. Headspace samples were also taken to determine CO_2 and CH_4 soil fluxes. Relative to upland soils, thermokarst soils were expected to release more CH_4 and less CO_2 during draining and promote more efficient microbial iron reduction during saturation. Initial results indicate that thermokarst soil does release more CH_4 and less CO_2 during draining than upland soil, which is undoubtedly related to faster soil drainage (~3x initial drainage rate) in the upland soil. This trend could also be partially attributed to prior adaptation of upland and thermokarst microbial communities to more oxic and oxygen-depleted conditions, respectively. Iron cycling – from reduction during saturation to oxidation during draining – was observed in both soil types, and the links between carbon and iron cycling are being evaluated in terms of organic electron donors and iron mineral-associated organic carbon. This column study will help constrain the relative importance and timing of aerobic respiration, anaerobic respiration through iron oxidation/reduction, fermentation, and methanogenesis on carbon cycling in Arctic soils undergoing redox transitions. This dataset will also inform integration of redox processes impacted by transport and changing oxygen availability into reactive transport models, such as PFLOTRAN, which are being coupled to terrestrial components of Earth system models.

Environmental Controls on Observed Spatial Variability of Soil Pore Water Geochemistry in Small Headwater Catchments Underlain with Permafrost

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Permafrost thaw in the Arctic is causing significant changes to landscape structure, hydrology, vegetation, and biogeochemistry. The integrated hydrogeochemical effect of these environmental changes are already apparent in the chemistry of the large Arctic rivers, where fluxes of carbon and nutrients are increasing, leading to enhanced nutrient loadings, with strong implications for the global carbon cycle. While the watershed areas of large Arctic rivers are vast, recent studies suggest that solute concentrations in these large rivers are likely controlled by solute generation processes occurring at much smaller scales. In this sense, changes in hydrogeochemistry in small Arctic catchments not only impact hydrogeochemistry at much larger scales, but also prognosticate the future hydrogeochemistry of larger Arctic rivers. While there is a rapidly growing body of literature focused on observing and understanding the impacts of Arctic warming on landscape structure, hydrology, vegetation, and biogeochemistry, relatively few studies directly address the existing spatial variability. In this study, we quantitatively evaluate the spatial variability of soil pore water geochemistry within two distinct catchments underlain with permafrost, and then seek to identify the source of the observed spatial variability. The soil pore water geochemistry of 18 locations spanning two small Arctic catchments were examined for spatial variability and its dominant environmental controls. The primary environmental controls considered were vegetation, soil moisture/redox condition, water/soil interactions and hydrologic transport, and mineral solubility. The sampling locations varied in terms of vegetation type and canopy height, presence or absence of near-surface permafrost, soil moisture, and hillslope position. As source areas for geochemical fluxes to the broader Arctic hydrologic system, geochemical processes occurring in these environments are particularly important to understand and predict with regards to such environmental changes.

Assessing Dynamic Vegetation Model Parameter Uncertainty Across Alaskan Arctic Tundra Plant Communities

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As the Arctic region moves into uncharted territory under a warming climate, it is important to refine the terrestrial biosphere models (TBMs) that help us understand and predict change. One fundamental uncertainty in TBMs relates to model parameters, configuration variables internal to the model whose value can be estimated from data. We incorporate a version of the Terrestrial Ecosystem Model (TEM) developed for arctic ecosystems into the Predictive Ecosystem Analyzer (PEcAn) framework. PEcAn treats model parameters as probability distributions, estimates parameters based on a synthesis of available field data, and then quantifies both model sensitivity and uncertainty to a given parameter or suite of parameters. We examined how variation in 21 parameters in the equation for gross primary production influenced model sensitivity and uncertainty in terms of two carbon fluxes (net primary productivity and heterotrophic respiration) and two carbon (C) pools (vegetation C and soil C). We set up different parameterizations of TEM across a range of tundra types (tussock tundra, heath tundra, wet sedge tundra, and shrub tundra) in northern Alaska, along a latitudinal transect extending from the coastal plain near Utqiaġvik to the southern foothills of the Brooks Range, to the Seward Peninsula. TEM was most sensitive to parameters related to the temperature regulation of photosynthesis. Model uncertainty was mostly due to parameters related to leaf area, temperature regulation of photosynthesis, and the stomatal responses to ambient light conditions. Our analysis also showed that sensitivity and uncertainty to a given parameter varied spatially. At some sites, model sensitivity and uncertainty tended to be connected to a wider range of parameters, underlining the importance of assessing tundra community processes across environmental gradients or geographic locations. Generally, across sites, the flux of net primary productivity (NPP) and pool of vegetation C had about equal uncertainty, while heterotrophic respiration had higher uncertainty than the pool of soil C. Our study illustrates the complexity inherent in evaluating parameter uncertainty across highly heterogeneous arctic tundra plant communities. It also provides a framework for iteratively testing how newly collected field data related to key parameters may result in more effective forecasting of Arctic change.

Effect of Slope Topography on the Above- and Below-ground Traits in Tundra Biome: Case Study at the Seward Peninsula

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Slope terraces are a widespread feature on the Seward Peninsula. These landforms affect the redistribution of snow during the winter season and control soil temperature and moisture regime, thus influencing vegetation and soil development. To study these mechanisms, we conducted research at one of such terraces at milepost 28 of the Teller Road. Our field activities included soil, vegetation, and snow surveys along a 70-meters long transect parallel to the terrace tread, biomass productivity assessment, decomposition experiment, and continuous measurements of the ground temperature and soil moisture at three points located in the rear, middle and front parts of the terrace. Our results showed mean annual ground temperature at the depth of 1.2 meters in 2019 gradually decreases from 1.9-4.2°C at the rear part to 0.1-0.5°C with a potential for a perennial frozen layer at the terrace's edge. Such a pattern in the ground thermal regime is most likely caused by the difference in winter temperature due to snow redistribution. The soil moisture regime is identified as Ustic at the rear and middle parts and Udic at the front of the terrace. Across the tread of the terrace vegetation changes from Mesic graminoid-herb meadow in the rear part to Cassiope dwarf shrub tundra in the middle and Ericaceous-lichen dwarf shrub tundra at the front. Aboveground bioproductivity increases from the rear (449.6 g/m^2) to the front part (1099.76 g/m^2) of the terrace. But, because of the differences in composition of plants communities, amount of annual litter biomass decreases from the rear to the frontal part. The highest rate of litter decomposition during the summer season occurs at the middle section of the terrace and the lowest – at the front. Processes of the organic stabilization were the lowest at the rear part of the terrace. A combination of all about mentioned factors and processes explain the pattern in soil sequence. The most developed soil profile (Ustic Haplocryols) can be found at the rear part of the terrace replaced with the Typic Humicryepts at the middle and Typic Dystrogelepts/Haplogelepts at the front. All of these processes also create the patterns of spatial variability of carbon budget and the greenhouse gases fluxes.

Dispersal and Fire Limit Arctic Shrub Expansion

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Arctic shrub expansion has been widely reported in recent decades, with large impacts on carbon budgets, albedo, and warming rates in high latitudes. However, predicting shrub expansion across regions remains challenging because the underlying controls remain unclear. Observational studies and models typically use relationships between observed shrub presence and current environmental suitability (bioclimate and topography) to predict shrub expansion, but such approaches omit potentially important demographic processes and non-stationary response of shrubs to changing climate. Here, we investigated controls on shrub expansion as part of the NGEE Arctic project. We used long-term high-resolution satellite imagery across Alaska and western Canada to show that observed shrub expansion has not been controlled by environmental suitability during 1984—2014, but rather can only be explained by accounting for seed dispersal and fire. These findings provide the impetus for better observations of recruitment and for incorporating currently underrepresented processes of seed dispersal and fire in land models to project shrub expansion and future climate feedbacks. Integrating these dynamic processes with projected fire extent and climate, we estimate that shrubs will expand into 25% of the non-shrub tundra by 2100, in contrast to 39% predicted using a relationship with increasing suitability alone. Thus, using environmental suitability alone likely overestimates and misrepresents the spatial pattern of shrub expansion and its associated carbon sink.

Climatic and Environmental Controls on Recent Arctic Tundra Shrubification

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Vegetation composition shifts, and in particular, shrub expansion across the Arctic tundra are some of the most important and widely observed responses of high-latitude ecosystems to rapid climate warming. These changes in vegetation potentially alter ecosystem carbon balances by affecting a complex set of soil–plant–atmosphere interactions. We synthesized the literature and found that shrub expansion is affected by several interacting factors including climate warming, accelerated nutrient cycling, changing disturbance regimes, and local variation in topography and hydrology. Under warmer conditions, tall deciduous shrubs can be more competitive than other plant functional types in tundra ecosystems because of their taller maximum canopy heights and often dense canopy structure. We also examined the role topography plays in determining shrub expansion by applying a coupled transect version of a mechanistic ecosystem model (*ecosys*) in a tundra hillslope site across the Kougarok watershed, Alaska. We found that intermediate soil water content in the mid-slope position enhanced mineralization and plant N uptake, thereby increasing shrub biomass. A simulation that removed topographical interconnectivity between grid cells resulted in (1) a 28% underestimate of mean shrub biomass and (2) over or underestimated shrub productivity at the various hillslope positions. Our results indicate that land models need to account for differences in plant traits that control competition and hillslope-scale coupled surface and subsurface hydrology to accurately predict current shrub distributions and future trajectories in Arctic ecosystems.

Impact of Short-term Warming on Carbon and Nitrogen Cycling Along the Plant-Soil Continuum

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The majority of plant biomass is located belowground in Arctic ecosystems, and plant roots are responsible for the uptake of nutrients that limit plant growth in these ecosystems. Despite performing a crucial role connecting primary producers to the soil, plant roots are relatively understudied in the Arctic and their functional response to rapidly warming climate is unknown. We therefore decided to assess whether one growing season of elevated temperature would have an impact on belowground carbon (C) and nitrogen (N) dynamics in the tundra. We conducted two field campaigns in Utqiaġvik, AK where we were able to sample Zero Power Warming Chambers deployed by NGEE Arctic. These chambers elevate air temperatures by around 4°C and surface soil temperatures by around 1°C during the peak growing season. To understand the impact of the warming treatment on both C and N dynamics, in 2018 we quantified the uptake of $^{15}N\text{-}NH_4$ from the soil by the arctic grass *Arctagrostis latifolia*. In 2021, we looked at the aboveground uptake of $^{13}C\text{-}CO_2$ by the sedge *Carex aquatilis*. Together, these experiments allow us to trace the path of N up from the soils through plant tissues as well the path of C downward from plant leaves, through roots, and into the rhizosphere. In 2018, we found that soil N and P availability increases significantly with warming, but biomass N and P pools of *A. latifolia* do not. Uptake of N by this grass species was not significantly impacted by warming, but we did see a strong relationship between soil NH_4 availability and uptake provided these variables were expressed in spatially explicit units (NH_4 per cm^3 soil & uptake per m fine root). In 2021, in addition to sampling plant tissues, our team also collected daily leaf samples, daily soil porewater samples, and measured soil microbial biomass at the end of a one-week incubation period. Preliminary observations from the 2021 campaign include the formation of iron-oxide plaques on root surfaces, indicating that oxygen (O) is flowing from the plant roots to the rhizosphere. Future analyses will quantify the transfer of recent photosynthate to soil porewater and the soil microbial community as well as allocation of this photosynthate within plant tissue. This research highlights the important role that interactions between plants, soils, and microbes play in determining local biogeochemistry.

Fine-scale Vegetation Composition and Structure Drives Variation in Spatial and Temporal Dynamics of Surface Albedo in Low Arctic Tundra

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Albedo, a measure of the solar reflectivity, is an important biophysical property of the land surface that influences local heating, regulates vegetation-atmosphere interactions and is a strong determinant of Earth's energy balance. In the Arctic, rapid climate warming is driving dramatic changes in vegetation distribution and land surface structure, including a rapid expansion of shrub and tree species into the Arctic tundra. This widespread replacement of vegetation species and structure is expected to have strong impacts on albedo, and as a result, on ecosystem energy balance. At the same time, Arctic vegetation distribution is strongly tied to the presence of permafrost, moisture and nutrient gradients, and fine-scale topographic features resulting in a high degree of spatial heterogeneity. This inherent variability combined with climate-driven changes in vegetation cover creates complex albedo responses in the Arctic. Traditional methods used to quantify albedo change and spatial patterns have been limited by their relatively low spatial resolution (e.g., > 250 m), requiring new, multi-scale observations to characterize the direction and rate of change in surface albedo. In this study, we address this need by combining remote sensing data across scales, from unoccupied aerial systems, high-resolution topography data, to piloted airborne and satellite observations to investigate the links between vegetation composition, structure, functional properties, and topographic features on the resulting spatio-temporal patterns of albedo in western Alaska. We used a time-series (2013 – 2020) Landsat albedo product across three watersheds located in the Seward Peninsula to investigate how sub-pixel patterns influence regional albedo. We observed strong regional albedo seasonality, but also significant differences in albedo patterns across the plant functional types, with tree and shrub species showing lower albedo than low-stature plants. In the winter, albedo is primarily a function of vegetation height, likely because taller vegetation, which is darker than the surrounding snow, extends above the snow layer. In the summer season, vegetation composition and topographic position, a strong driver of tall shrub distribution, were more important for explaining albedo variation than vegetation structure. Our results suggests that changes in vegetation composition and structure will create increasingly complex albedo patterns across the Arctic, and our dataset can be used to inform and benchmark process models predictions of Arctic albedo.

Near-Surface Hydrology and Soil Properties Drive Heterogeneity in Permafrost Distribution, Vegetation Dynamics, and Carbon Cycling in a Sub-Arctic Watershed

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Discontinuous permafrost environments exhibit strong spatial heterogeneity in subsurface thermal states, vegetation cover, and carbon fluxes, with sharp transitions that occur at scales too small to be driven by weather forcing or to be captured by Earth System Models. Here we analyze – using field observations and an ecosystem model – the effects of observed spatial heterogeneity in soil and vegetation properties, hydrology, and thermal dynamics on ecosystem carbon dynamics in a watershed on the Seward Peninsula in Alaska. First, we quantify the controls on soil thermal regimes across the watershed using a dense network of distributed temperature profiling systems (DTP). The DTP data indicates that the soil thermal regimes are primarily driven by snow depth and co-vary with vegetation type with near-surface permafrost and talik present under graminoid and shrub covered area, respectively. Further, we evaluate the mechanisms driving this co-variability and its impact on carbon dynamics by applying a Morris global sensitivity analysis (GSA) to a process-rich, successfully tested terrestrial ecosystem model, *ecosys*. The GSA outputs cover the observed ranges of soil temperatures, soil moisture, and surface CO_2 fluxes observed in the watershed and confirm that landscape heterogeneity has a strong impact on soil temperatures, permafrost distribution, and vegetation composition. Snow depth, O-horizon thickness, and near-surface water content control the soil thermal regime more than an air temperature gradient corresponding to a 140 km north-south distance. High shrub productivity is simulated only in talik (perennially unfrozen) soils with high nitrogen availability Through these effects on PFT and permafrost dynamics, landscape heterogeneity impacts ecosystem productivity. We find that model runs with near-surface taliks have higher microbial respiration (by 78.0 gC m^{-2} yr^{-1}) and higher net primary productivity (by 104.9 gC m^{-2} yr^{-1}) compared to runs with near-surface permafrost, and simulations with high shrub productivity have outlying values of net carbon uptake. We explored the prediction uncertainty associated with ignoring observed landscape heterogeneity and found that watershed net carbon uptake is three times larger when heterogeneity is accounted for. Our results highlight the complexity inherent in discontinuous permafrost environments and demonstrate that missing representation of subgrid heterogeneity in TEMs could bias predictions of high-latitude carbon budget.

Integrating Arctic Vegetation and Biogeochemical Processes into the E3SM Land Model

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Earth system models are a critical tool for projecting future changes in climate and ecosystems. A major goal of the NGEE Arctic project is to integrate improved scientific understanding of Arctic systems into the Energy Exascale Earth System Model (E3SM) to connect scientific discoveries from observations, experiments, and detailed modeling of the Arctic into global-scale predictive models. New understanding of Arctic processes is being incorporated into hydrological, physical, biogeochemical, and vegetation process modules in the E3SM Land Model (ELM) through multiple integrative modeling efforts as part of NGEE Arctic Phase 3. I will highlight recent progress in two of these integrative modeling efforts. First, improvements to ELM with the goal of better representing vegetation traits by integrating nine tundra-specific plant functional types (PFTs); several that are new to the model, including nonvascular mosses and lichens, graminoids, forbs, and shrubs of various height classes as well as a nitrogen fixing alder shrub. These developments leverage extensive field sampling of vegetation species distributions and biomass and are now being integrated with remote sensing of vegetation communities and traits to configure ELM model simulations of tundra vegetation carbon and nutrient cycling across the Seward Peninsula of Alaska. Second, we have implemented new soil biogeochemical capabilities with the goal of better representing greenhouse gas production across complex tundra landscapes. We have developed a reaction network in the geochemical simulator PFLOTRAN including pH dynamics, iron redox cycling, oxygen consumption, methanogenesis, and soil nitrogen cycling informed by experimental and field measurements of tundra soil processes. Furthermore, we have coupled this reaction network to ELM representation of soil organic matter decomposition within a coupled ELM-PFLOTRAN framework, allowing fully integrated simulations of complex biogeochemical cycling within E3SM. Altogether, these developments translate discovery science from a range of observations, experiments, and detailed modeling studies within the NGEE Arctic project into concrete improvements in E3SM modeling capabilities.

Arctic Alder Nodule Microbe: Insights into Nitrogen Fixation

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This project uses state of the art sequencing and imaging technologies to resolve complex plant-microbe interactions governing the nitrogen fixation in tundra biomes to better inform efforts to decipher arctic nitrogen cycling. Plant roots are home to beneficial microbes where microorganisms help plants to obtain nutrients, tolerate stress and sustain growth. Nitrogen (N) fixation is a common mutualistic symbiosis where the plant provides the N-fixing bacteria with sugars and a variety of minerals, and the bacteria provide the host with N. We investigated the nodule microbiome of alder *Alnus viridis* spp. *fruticosa*, an N-fixing deciduous shrub and an important contributor to N-cycling in the tundra. *Frankia alni* and its relatives form a symbiotic relationship exclusively with trees in the genus *Alnus* but this actinorhizal symbiosis is not as well characterized as the agriculturally important legume-rhizobia symbiosis, especially in the Arctic. The Kougarok study site is situated in the Seward Peninsula, AK. At this location alder is found as two distinct communities: short and dispersed alder growing in lowland areas (“alder savanna”) and tall alder growing as dense, tall shrublands along the rocky ridge of the hillslope (“alder shrubland”). We collected root free soil samples next to the plants and nodules from both alder communities. We extracted and sequenced the whole community DNA from both nodules and surrounding soils resulting several hundred metagenome assembled genomes (MAGs) and viral genomes (vMAGs) of bacteriophages. We coupled metagenomics with analysis of intra-nodule biochemistry via synchrotron fourier transform infrared (SR-FTIR) spectral imaging at the Berkeley Infrared Structural Biology beamline of the Advanced Light Source. The alder microbiome was dominated by a novel *Frankia* strain. Both alder communities contained non-*Frankia* bacteria but alder shrubland had a higher bacterial diversity than alder savanna. Non-*Frankia* bacteria in alder nodules contained carbohydrate degradation genes involved in hemicellulose, mannose and xylose degradation. Bacteriophages associated with alder nodule microbiome carry carbohydrate degradation genes specific to cellulose, xylose and pectin degradation. SR-FTIR analysis showed that despite differences in microbiomes alder nodules both communities had similar biochemical in the composition at a functional group level where metabolites involved in N-fixation was dominating the chemical spectra. However, we also observed strong intra-plant and -nodule variation which was decoupled from N-fixation processes. Arctic alder nodules house a diverse microbiome and has a rich biochemical composition. This diversity can be associated with plant growth and inputs of biologically-available N into nutrient-poor Arctic ecosystems.

Integrating Field Observations and Multi-scale Remote Sensing to Understand Tall Shrub Distribution in Arctic Tundra

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The Arctic region has experienced some of the most rapid climate warming on Earth. In response to this warming and associated permafrost thaw, an increase in the abundance of tall shrubs (those that can potentially grow greater than 2 m tall) has been observed across the Arctic, with significant implications on Arctic biodiversity, energy balance, and the biogeochemical cycling of carbon, water, and nutrients. However, uncertainties persist in quantifying the primary drivers of the distribution and rate of shrub expansion in Arctic tundra. While warming temperatures and permafrost thaw are expected to be a key driver, shrub distribution is also likely limited by other biotic and abiotic factors that do not favor their growth (e.g., topographic control and soil moisture). Changes in these limiting factors could have larger or more direct impacts on shrub expansion. In this study, we combined ground observations and multi-scale remote sensing data, including occupied aerial system (UAS; 5 cm), NASA's Airborne Visible / Infrared Imaging Spectrometer (AVIRIS-NG; 5 m), ArcticDEM (30 m), high-resolution down-scaled climate data (60 m), and model simulated soil data (500 m), to investigate the drivers and limits of tall shrub distribution in Western Alaska. We first mapped the fractional cover (FCover) of two key tall shrub genera (alder and willow) using AVIRIS-NG imagery collected on the Seward Peninsula and a vegetation cover scaling approach that we have developed for AVIRIS-NG. We then combined the alder and willow FCover maps with topographic, climate, and soil moisture data to investigate the primary determinants of tall shrub distribution. We found that topography is a primary control on tall shrub distribution in the Arctic. The distribution of alder is strongly limited by elevation and slope, with a higher cover found within the 100 - 300 m, MSL elevational band. In contrast, the distribution of willow is more closely tied to surface wetness. To understand the biological mechanisms of these differences, we further examined their biochemical and physiological traits, and found that willow has a lower instantaneous water-use efficiency than alder, suggesting why willow is found in wetter conditions. These findings suggest that different shrub species may respond to the climate change differently. Improved understanding of the controls on tall shrub distribution is important to accurately forecast the response of arctic ecosystems to current and future climate change.

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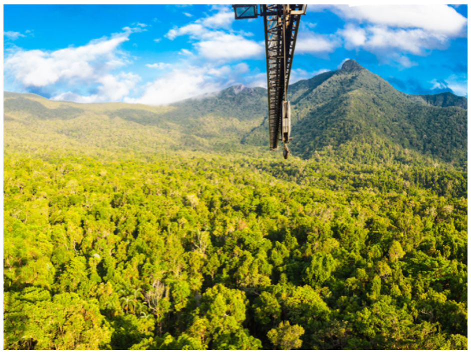

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ENVIRONMENTAL SYSTEM SCIENCE

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Title: Do tropical forest trees have limited water sources? Plant water sourcing depth across the neotropics.

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Project Lead Principal Investigator (PI): Jeffrey Chambers, Berkeley Lab
BER Program: ESS
Project: NGEE-Tropics (led by Berkeley Lab)
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract:
Plant water availability and sourcing depth is central to understanding vegetation responses and coping mechanisms to water stress and increases in drought. Stable isotopes of water ($\delta^{18}O$ and $\delta^{2}H$) can be powerful tracers to investigate effective tree rooting depth when combined with site- and species-specific information like soil type, soil water and water table dynamics, and plant hydraulic traits. Yet, such studies are limited in the humid tropics, especially considering that it is difficult to time water isotope sampling with a significant dry-down which creates an isotopic separation of water sources across soil profile. Moreover, some of the foundational water isotope work conducted in the tropics generally relied on only one isotope tracer, which limits Bayesian and other mixing-model frameworks aimed at quantifying source water contributions. As a first step towards overcoming some of these challenges, we conducted repeated stem and soil water sample collections at several core NGEE-Tropics sites in the neotropics, which also have long-term hydrological or ecological data. These sites include the ZF2 ecological experiment station in the central Amazon, Brazil and Parque Natural Metropolitano and Barro Colorado Island in Panama. Other sites for which data has been collected opportunistically include the San Lorenzo site in Panama, and Mulehole in India. While it is thought that shallow soil water is sufficient to sustain forests during the dry season, here we summarize recent finding that for the ZF2 and BCI sites, the forest stand generally shifts to deeper soil water during periods with limited rainfall, suggesting that at least for some canopy-dominant species, which may drive ET patterns, deep soil water help trees cope with or all together avoid water stress. Other related work has reported that species across a rainfall gradient in Panama exhibit very little difference in leaf hydraulic traits within sites (see WP 1.2). We also report on preliminary data including the ecohydrological dynamics of soil moisture and groundwater for ZF2, soil moisture for BCI and ELM-FATES based modeling of soil moisture dynamics in Paracou, French Guiana. We discuss steps forward regarding water isotope analysis of samples collected across neotropical sites during dry periods in 2019-2022. This includes synergies with WP 1.3 linking leaf spectral and trait data to plant water isotope data, and MODEX efforts to validate inverse rooting-depth models of pantropical sites.

Title: Relationships between plant hydraulic traits, gas exchange, and species demography in Panama

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Project Abstract:

Climate change is impacting community demographics of tropical forests globally, but the underlying drivers and mechanisms of these responses are not understood. We investigated how species' physiological traits were associated with demographic trends and changes in climate over a 30-year monitoring period at Barro Colorado Island (BCI), and across an additional 71 sites with species composition inventories distributed along a moisture gradient across Panama. For all sites we collected associated species' trait data from published sources. The community dynamics of evergreen tropical tree species at BCI exhibited the expected life history trade-off of species having high mortality rates, fast growth rates, and high recruitment rates on one end of the continuum, and species on the other end of the continuum showing the opposite patterns. Xylem vulnerability to cavitation was the only tested trait that correlated with the life-history strategies, with fast-living species having more vulnerable xylem than slow-living species. The only significant relationship between demographic rates and climate variables was with temperature and mortality; hotter years exhibited higher mortality. However, despite substantial climate variability, there were no significant temporal changes in community weighted physiological traits at BCI over the monitoring period. Patterns across the regional transect, in contrast, exhibited large variation in response to local climate, with some particularly surprising hydraulic- and carbon-based trait trade-offs. These results suggest that forest communities adapt to local site conditions over longer-time scales than monitored at BCI, and indicate that for the forest at BCI, community-trait shifts may be slower than the rapid and variable changes in climate, potentially resulting in rising mortality as temperature increases.

Title: Survey Derived Gas Exchange Data Identify Diurnal Patterns in Leaf Level Water Use Efficiency and Improve Model Representation of Stomatal Function in Tropical Forests

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Project Abstract:
A primary source of uncertainty in Earth system model (ESM) projections of terrestrial carbon and water cycling is the relationship between CO_2 assimilation (A) and water loss via stomatal conductance (g_s). A common framework for modeling this relationship relates A to g_s over environmental conditions (temperature, CO_2, irradiance, and humidity) and is governed by two terms, the stomatal slope (g_1) and intercept (g_0). Given their importance in determining the relationship between forest productivity and climate, an accurate and mechanistic understanding of the g_1 and g_0 parameters is crucial. In this study, we assess possible physiological and mechanistic controls on the estimation of g_1 and g_0 using both diurnal gas exchange surveys and leaf level response curves for six tropical broadleaf evergreen tree species across a full range of leaf phenological stages. We found that g_1 estimated from curves was on average 50% less than g_1 estimated from survey data. We also show that while g_0 varied significantly between leaves of different phenological stages, this effect was generally not observed for g_1. While some species groups exhibited variable g_0 or g_1 with phenological stage, among species groups there was no consistent pattern of change in g_0 or g_1 with phenological stage. We also identified a diurnal trend associated with g_1 and g_0 that significantly improved model projections of diurnal trends in g_s. These results suggest that to improve the accuracy of modeled g_s in tropical forests, we should investigate the mechanism responsible for variation among species and across diurnal patterns.

Title: Stem Respiration and Growth in a Central Amazon Rainforest

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Project Abstract:
Tropical forests cycle a large amount of CO_2 between the land and atmosphere, with a substantial portion of the return flux due to tree respiratory processes. However, *in situ* estimates of woody tissue respiratory fluxes and carbon use efficiencies (CUE_W) and their dependencies on physiological processes including stem wood production (P_w) and transpiration in tropical forests remain scarce. Here, we synthesize monthly P_w and daytime stem CO_2 efflux (E_S) measurements over one year from 80 trees with variable biomass accumulation rates in the central Amazon. On average, carbon flux to woody tissues, expressed in the same stem area normalized units as E_S, averaged 0.90 ± 1.2 μmol m^{-2} s^{-1} for P_w, and 0.55 ± 0.33 μmol m^{-2} s^{-1} for daytime E_S. A positive linear correlation was found between stem growth rates and stem CO_2 efflux, with respiratory carbon loss equivalent to $15 \pm 3\%$ of stem carbon accrual. CUE_W of stems was non-linearly correlated with growth and was as high as 77-87% for a fast-growing tree. Diurnal measurements of stem CO_2 efflux for three individuals showed a daytime reduction of E_S by 15-50% during periods of high sap flow and transpiration. The results demonstrate that high daytime E_S fluxes are associated with high CUE_W during fast tree growth, reaching higher values than previously observed in the Amazon Basin (e.g. maximum CUE_W up to 77-87%, versus 30-56%). The observations are consistent with the emerging view that diurnal dynamics of stem water status influences growth processes and associated respiratory metabolism.

Reference: Jardine K, Cobello L, Teixeira L, East M, Levine S, Gimenez B, Robles E, Spanner G, Koven C, Xu C, Warren J, Higuchi N, McDowell N, Pastorello G, Chambers J (2022). Stem respiration and growth in a central Amazon rainforest, *Trees,* 20:1-4.

Title: Overlooked Aboveground Biomass Losses in Tropical Forests

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BER Program: ESS

Project: NGEE-Tropics (led by Berkeley Lab)

Project Website: https://ngee-tropics.lbl.gov/

Project Abstract:

Tree mortality is typically considered as the only carbon output in forest systems. However, a pervasive but commonly neglected source of biomass loss is the damage to living trees (i.e., branch fall, trunk partial breakage, and/or standing wood decomposition). The dry, living, aboveground biomass (AGB) estimated from the trunk diameter of trees that are damaged but remain alive are not counted as losses in traditional forest inventories. Here we use 28 annual mortality and damage censuses to quantify AGB loss via damage on living trees and compare its relative contribution to total AGB loss (mortality + damage) in seven tropical forest plots of the ForestGEO network in the Neotropics (Amacayacu, Colombia; Barro Colorado Island, Panamá; Yasuní, Ecuador) and Asia (Fushan, Taiwan; Huai Kha Khaeng, Thailand; Khao Chong, Thailand; Pasoh, Malaysia). We found that almost half of total AGB losses were due to damage to living trees. The contribution of damaged trees to total AGB losses was highly variable across sites and over time, ranging from 13% in a lowland dipterocarp forest in Malaysia to 86% in a typhoon-prone forest in Taiwan. Our results show the importance of quantifying tree-level biomass loss through crown and trunk damage for obtaining more accurate estimates of tropical forest carbon stocks and fluxes.

Title: Simulating Environmentally Sensitive Tree Recruitment in Vegetation Demographic Models

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Project Abstract:
Vegetation demographic models (VDMs) endeavor to predict how global forests will respond to climate change. This requires simulating which trees, if any, are able to recruit under changing environmental conditions. We present a new recruitment scheme for VDMs in which functional-type-specific recruitment rates are sensitive to light, soil moisture, and the productivity of reproductive trees. We evaluate the scheme by predicting tree recruitment for four tropical tree functional types under varying meteorology and canopy structure at Barro Colorado Island, Panama. We compare predictions to those of a current VDM, quantitative observations, and ecological expectations. We find that the scheme improves the magnitude and rank order of recruitment rates among functional types and captures recruitment limitations in response to variable understory light, soil moisture, and changing precipitation regimes. Our results indicate that adopting this framework will improve VDM capacity to predict functional-type-specific tree recruitment in response to climate change, thereby improving predictions of future forest distribution, composition, and function.

Title: The Distribution of EcM Trees in Lowland Tropical Forests

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Project Abstract:
A lot has recently been written about the global distribution of plant nutrient acquisition strategies related to symbioses between fungi and trees, typically asserting that lowland tropical forests are dominated by plants with arbuscular mycorrhiza (AM) symbioses while ectomycorrhiza (EcM) symbioses are rare or absent. Climatic effects on decomposition rates and local variation in soil quality are considered the main drivers of the global and the local, fine-scale pattern of plant-fungi symbiotic distributions. AM is predicted to dominate at low latitudes and in areas with high soil quality while at high latitudes, and in areas with low soil quality, EcM is predicted to dominate. Using data from a pantropical network of forest dynamics plots, we show that the three major areas of lowland tropical forest differ in their plant-symbiont composition. Most lowland Asian rainforests are dominated by EcM, primarily species of the Dipterocarpaceae. African forests are dominated by mixtures of ectomycorrhizal species, including large expanses of monodominant forests. With the exception of small areas in the Guiana Shield and some white-sand habitats, South American lowland rainforests, including the Amazon Basin, are dominated by AM symbioses and are largely devoid of EcM species. These major differences in plant-symbiosis relationships are unrelated to soil fertility or climate at the pantropical scale. Historical biogeography and unique patterns of diversification within the three regions have resulted in dramatically different forest compositions and putative nutrient-acquisition strategies. Earth System Models treat lowland tropical forests as one biome. Differences in patterns of plant-fungi symbiosis across the lowland tropics have important consequences for carbon uptake and storage in response to global environmental change.

Title: Climate Warming Projected to Cause a Large Increase in Amazon Windthrow Disturbance This Century

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Project: NGEE-Tropics (led by Berkeley Lab)
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Project Abstract:
Forest mortality caused by convective storms (windthrow) are major disturbances in the Amazon, which shape forest structure and affect the regional carbon balance. However, the linkage between windthrow at the surface and convective storms in the atmosphere is poorly understood. In addition, the current Earth system models (ESMs) lack mechanistic links between convective wind events and tree mortality. Here we show that a simple proxy that is well simulated by global climate models (GCMs) – convective available potential energy (CAPE) – explains 57% of the variance in the spatial density of windthrow events encompassing 30 years in the Amazon. Using remote sensing and climate reanalysis data, this relationship builds connections between strong convective storms and forest dynamics for the first time in the Amazon. An analysis of 10 GCMs predicts a significant increase of CAPE with a warming climate, and our models using CAPE project a 65 ± 43% increase in windthrow density over this century. These results augur significant changes in tropical forest composition and carbon-cycle dynamics under climate warming.

Title: Key Parameters under Varying Phosphorus Supply in the Nutrient-enabled ELM-FATES

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Project Website: https://ngee-tropics.lbl.gov/

Project Abstract:

Demographically structured vegetation models have a large number of input parameters, which complicates model development and calibration. Quantifying the impact of each parameter on model outputs and identifying key influential parameters are necessary to understand model behavior at various spatial-temporal scales. In this study, we conducted a comprehensive sensitivity analysis to diagnose influential parameters in the Energy Exascale Earth System Model (E3SM), land model (ELM) coupled to the nutrient-enabled Functionally Assembled Terrestrial Ecosystem Simulator (ELM-FATES). We used the Luquillo Experimental Forest site in Puerto Rico as a testbed to quantify the global sensitivities of model outputs (including carbon fluxes and above-ground biomass) to 43 model parameters. Since the phosphorus is generally limited in tropical forest ecosystems, we examined impacts of less phosphorus supply on the ELM-FATES parameter sensitivity. We designed two scenarios. In scenario 1, we used the climate data during the time period of 1995-2014 and high phosphorus supply to drive the model. In scenario 2, we used lower phosphorus supply together with the same climate data. We identified key parameters by using 1,000 model simulations of each scenario together with the Sobol' sensitivity indices from chaos. Overall, specific leaf area at the top of canopy and leaf N:C ratio were found to be the two most important parameters for simulated carbon stocks and fluxes. When phosphorus supply was low, the leaf C:P ratio became a more influential parameter for the above-ground biomass and gross primary production.

Title: Coupled Modeling of Hillslope Hydrology and Ecosystem Dynamics at Manaus and BCI

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Project: NGEE-Tropics
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Project Abstract:
Tropical forests play essential roles in the coupled land-atmosphere system by contributing to a large fraction of precipitation through evapotranspiration. Combined climate change and topography are likely to have considerable and diverse impacts on plant water availability, with consequential effects on vegetation dynamics and the regional and global water cycles. We have developed an integrated model that couples E3SM Land Model (ELM), an ecosystem dynamics model (FATES), and a three-dimensional hydrology model (ParFlow) to explicitly resolve hillslope topography and subsurface flow for a better understanding of the processes that drive plant water availability and tropical forest dynamics. Numerical experiments are conducted at Barro Colorado Island, Panama, and the Asu catchment, Manaus. Differing in terrain features and rainfall seasonality, the two sites provide useful testbeds for evaluating the coupled model. Machine learning-based surrogate models are built to help calibrate ELM–FATES–ParFlow based on multiple observations, including measured soil moisture, groundwater table, energy and carbon fluxes, and forest inventory data. Experiment results are analyzed to identify the main physical processes that drive the observed forest structure and dynamics and to study the modulation of hillslope processes on how drought affects plant water availability and vegetation.

Title: Soil moisture thresholds explain a shift from light-limited to water-limited sap velocity in the Central Amazon during the 2015-16 El Niño drought

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Project Abstract:
Transpiration is often considered to be light- but not water-limited in humid tropical rainforests due to abundant soil water, even during the dry seasons. The record-breaking 2015-16 El Niño drought provided a unique opportunity to examine whether transpiration is constrained by water under severe lack of rainfall. We measured sap velocity, soil water content, and meteorological variables in an old-growth upland forest in the Central Amazon throughout the 2015-16 drought. We found a rapid decline in sap velocity (-38% ± 21%, mean ± SD.) and in its temporal variability (-88%) during the drought compared to the wet season. Such changes were accompanied by a marked decline in soil moisture and an increase in temperature and vapor pressure deficit. Sap velocity was largely limited by net radiation during the wet season; however, it shifted to be primarily limited by soil moisture during the drought. The threshold in which sap velocity became dominated by soil moisture was at 0.33 m^3/m^3 (around -150 kPa in soil matric potential), below which sap velocity dropped steeply. Our study provides evidence for a soil water threshold on transpiration in a moist tropical forest, suggesting a shift from light limitation to water limitation under future climate characterized by increased temperature and an increased frequency, intensity, duration and extent of extreme drought events.

Title: Importance of fire for functional biogeography across tropics

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Project Abstract:
Fire regimes are changing over much of the world. Fire risk has already increased across much of the tropics. Projecting the impact of these changes in global scale simulation requires that we are able to capture and understand how fire acts as a driver of biogeography. Utilizing the Functionally Assembled Terrestrial Ecosystem Simulator (FATES), a size-structured Vegetation Demographic Model, with the fire behavior and effects module SPITFIRE, we test how various fire regimes and contrasting fire tolerance plant traits interact to determine tropical biogeography of forests and grasses. Observations demonstrate that geographic variability in bark thickness is explained in part by burned area, with frequently burned areas having trees adapted with thicker bark. Fire tolerance strategy in FATES is based on tree bark thickness, crown size and foliage resistance to heat, which are key fire-tolerance traits across woody plants. Simulations demonstrate reasonable productivity and capture observed patterns of aboveground biomass for the recent historical period. Burned fraction from the model is over predicted in areas with grass dominance, but resulting biogeography of fire-tolerant thick bark trees and -intolerant thin bark trees correspond to observations across the tropics. Comparisons of size-based fire mortality show that the fire-tolerant thick bark trees escape mortality through height and fire resistant traits more effectively than the thin bark trees. Drier fuels in simulation are shown to promote increased burning, an expansion of grass and thick bark tree area and loss of area for fire-intolerant thin bark trees. Conversely simulations without fire result in exclusive dominance of the thin bark tree, which is less resource expensive compared to the thick bark tree. These results suggest that thin bark forests are vulnerable to increased fire. Our ability to capture the connection between active fire and plant's fire tolerance strategies in determining biogeography provides an essential tool for assessing the vulnerability and resilience of these critical carbon storage areas under changing conditions across the tropics.

Title: A Nutrient Enabled Demographic Ecosystem Model - FATES-ELM-CNP - Evaluation and Parametric Sensitivity at a Tropical Testbed

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Project Abstract:
Nitrogen and phosphorus play an important role in modulating global vegetation dynamics. Earth system models have shown that nutrient availability impacts projections of the global carbon sink. It has also been shown that terrestrial biosphere models that represent vegetation size, function and age structure, capture key processes that drive accurate and representative projections of forest demographics that traditional big-leaf models cannot. The Functionally Assembled Terrestrial Ecosystem Simulator (FATES) is a terrestrial vegetation model that is coupled with the Energy Exascale Earth System's Land Model (ELM). It can resolve plant growth, competition, mortality, recruitment and disturbance through a size, type and age structured scaling approximation. Until recently, these processes had been mediated solely through an evaluation of the plant's carbon balance. Here we present an updated version of the FATES-ELM model that accounts for the cycling of nitrogen and phosphorus between the vegetation and the soil microbiome, as well as the limitations that nutrient availability imparts on plant growth and dynamics. We evaluate the model at a tropical testbed site at Barro Colorado Island in Panama, using observations to constrain model parameters. We evaluate model hypotheses with a focus on the plant acquisition of mineralized nutrients, as well as their modulation of construction costs under nutrient limitations.

Title: The NGEE-Tropics Data Archive and Data Curation Activities

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Project Lead Principal Investigator (PI): Jeffrey Chambers, Berkeley Lab
BER Program: ESS
Project: NGEE-Tropics (led by Berkeley Lab)
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract:
The NGEE-Tropics Data Archive supports and stores ecological, hydrological, micrometeorological, and remote sensing data from tropical forests used to advance scientific understanding and to improve model behavior for these ecosystems. This includes providing data access for current and future research teams, evaluation of data packages being published for completeness, generation of digital object identifiers (DOIs), and supporting results from data quality assurance and quality control (QA/QC) activities for the project. Since 2016, the NGEE-Tropics team has collected data from 21 sites across the tropics, data which was foundational to studies at site, regional, and pantropical scales. Current NGEE-Tropics Archive holdings include 96 public data packages, containing, for instance, leaf related data, including variables such as leaf mass area, leaf respiration, phenology, and water potential, and soil data encompassing soil chemical composition, water content, and temperature, and also includes data on related to sap flow, meteorological measurements, tree mortality, root data, and model codes and outputs. A review of the metadata quality is performed prior to publication, and whenever suitable, our metadata reporting templates (FRAMES) allow researchers to provide file-, measurement-, and experiment-level metadata to accompany their data. Data QA/QC activities are also an integral part of the data-related activities for NGEE-Tropics, including, for instance, micrometeorological datasets prepared and now available for sites in Panama, and more recently sites in the Brazilian and Peruvian Amazon, including collaborative work on data from the partner LBA Project. The NGEE-Tropics Archive provides a tailored user experience in creating and validating these datasets, while also synchronizing and making these datasets also available in the ESS-DIVE Archive, aiming at the long-term preservation of access to these data. Several of these datasets are already being used in empirical and synthesis studies of tropical forests and also for ecosystem modeling efforts through the NGEE-Tropics Functionally Assembled Terrestrial Ecosystem Simulator-FATES model.

The impact of soil hydrological parameters on vegetation dynamics

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Project: NGEE-Tropics
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Infiltration is an important hydrologic parameter because it represents a primary control on the amount of water available for plant uptake as well as streamflow. However, few of these measurements exist due to the challenges associated with setting up and monitoring the necessary equipment. This is particularly true in remote areas of the tropics. As a result, state-of-the-art models used to model vegetation hydrodynamics are often poorly calibrated. We address this issue by using 12-months of sub-daily infiltration observations from a percolation flux meter to run an inverse model simulation within the HYDRUS 1D model at an old growth Amazon forest site near Manaus, Brazil. The site has a high clay content soil, yet is well-drained making it a challenge for most texture-based hydraulic models. Next, we are planning to use the calibrated hydrological parameters from HYDRUS in the DOE-sponsored vegetation dynamics model, the Functionally Assembled Terrestrial Simulator (FATES), to estimate plant hydrodynamics and vegetation dynamics within this ecosystem. We will compare the calibrated hydrological parameter results to a base case where the standard pedotransfer function in FATES is used. The results will be used to estimate potential biases when using the standard method from similar forested sites within the tropics. Research outcomes are aimed at improving model parameters employed within dynamic vegetation models and encouraging better precision with calibration techniques.

Using Machine Learning to Extend High-resolution Integrated Hydrology Models to River Basin Scales

Ethan Coon,[1] Dan Lu,[1] Scott Painter,[1] Carl Steefel,[2] Dipankar Dwivedi,[2] Xingyuan Chen[3], David Moulton[4] & the ExaSheds Team

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Project Lead Principal Investigator (PI): Carl Steefel and Scott Painter

BER Program: Other (Data Management)

Project: ExaSheds Project

Project Website: https://exasheds.org/

Project Abstract: Many of the impacts of climate and land use change are felt through the water cycle. Water availability, quantity, and quality are currently volatile, and ongoing change only reduces predictability. A predictive understanding of the impacts of these changes requires capability that operate across scales; while many of the processes governing the water cycle occur in watersheds at scales from 10s-100s of meters (macrotopography, land cover and land use variation), these processes must be integrated across full river basins (100s of kilometers) to determine their effect on society and the water cycle.

The ExaSheds project is developing a novel capability to address this scaling problem and thereby advance watershed system understanding. We have embraced a hybrid methodology, bringing together Machine Learning (ML) and process-rich simulations using high performance computing. The combined capability is fundamentally hierarchical, multiscale, and organized by watersheds, the natural unit for integrating water impacts. The goal is a general simulation capability that can be used by scientists and their stakeholder partners to advance understanding of regional-scale water cycles under future climates and conditions.

This talk describes progress toward ExaShed's vision of an ML-enabled strategy for scaling process-based models to river basin scales, focusing initially on stream discharge. We leverage ML to build surrogate models for high-resolution ATS models of individual watersheds within the larger basin. These surrogate models take as input time series of meteorological forcing and incoming flow from watersheds upstream as well as static attributes of the watershed. We are using current-day and future meteorological forcings downscaled by ML techniques from climate projections in forward simulations to train the surrogate models. Once trained using a

few years forcing data, the surrogate models can be used to invert for uncertain model parameters, extend the simulations to decadal time scales over large basin scales, and address scenario uncertainty associated with the future climate and land-use changes. The resulting modeling framework leverages the strengths of both data-driven and process-based modeling approaches – computationally feasible, large-scale predictions that maximize predictive power under current conditions while being robust to shifts to unprecedented future conditions.

Title: **Pore to Core: Linking Soil Organic Carbon Protection Mechanisms to Ecosystem CO2 Fluxes in Response to Varying Antecedent Soil Moisture Conditions**

Vanessa Bailey[1], Ben Bond-Lamberty[2], Jianqiu Zheng[1], and Kaizad Patel[1]

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BER Program: ESS

Project Lead Principal Investigator (PI): Vanessa Bailey

Project: PNNL Project

Project Website:

Project Abstract: The persistence of soil organic carbon in soils is a function of an integrated set of protection mechanisms, encompassing physical occlusion, chemical composition, and microbial competencies. Understanding how these three mechanisms intersect to protect carbon has been the focus of several years of research on this project; we have focused particularly on how antecedent drought and flood change the chemical forms and distribution of carbon through soil pores. These changes to pore-scale carbon chemistry and accessibility have then been assessed through the microbial production of carbon dioxide at the soil core scale.

We have used these experiments to improve our representations of carbon dioxide emissions from soils in response to extreme wetting and drying, with specific attention given to physical controls on microbial proximity to substrate and diffusion limitations. These findings have both informed process-rich simulation models and conceptual models of the contributions of physical occlusion and chemical composition to C longevity.

The third major leg of this project has been a series of data syntheses. These have, over the duration of this project, examined the importance of moisture, temperature, and geographic location to overall carbon fluxes, and assessed the fidelity of process models at a variety of spatial and temporal scales. These analyses have drawn connections between regional carbon distribution, carbon dioxide fluxes, and core-scale experimental conditions.

We summarize our advances toward a process-rich understanding of how SOC is decomposed as a result of pore-scale changes in SOC physical protection under varying antecedent moisture conditions.

The Influence of Soil Moisture and Tree Evapotranspiration on an Urban Microclimate

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Project Lead Principal Investigator (PI): Melanie Mayes

BER Program: ESS

Project: Biogeochemical cycling along the urban interface

Project Website: n/a

Project Abstract:

A highly uncertain part of predicting microclimate in urban environments involves natural ecosystem components, i.e., soils and plants, which vary with degree of urbanization. Richer Americans enjoy more greenery in their environments than lower-income communities, while neighborhoods with a majority of people of color have lower tree canopy compared to majority white communities. Further, people of color are more likely than whites to experience the urban heat island effect. The goal of this project is to understand how temperature and relative humidity in urban environments are affected by the activities of plant evapotranspiration and soil moisture. We hypothesize that soil moisture, the extent of impervious surfaces, and tree canopy will influence local microclimate; specifically, low soil moisture, high percentages of impervious surfaces, and low extent of tree canopy will cause more intense heating in the summer and more intense cooling in the winter. Additionally, high relative humidity can exacerbate the heat index and make people feel less comfortable. We are choosing a single site for a coupled model-experiment investigation by implementing a representativeness analysis over the eastern U.S. Initial factors under consideration are % canopy, impervious surfaces, soil moisture, albedo, summer precipitation, temperature, and relative humidity. This investigation will inform site choice by identifying a site that is broadly representative of other medium and large cities in the eastern U.S. Then, using the geospatial information from the analysis coupled with social data such as population density, race, and income, we will choose paired sites with contrasts in tree canopy, imperviousness, and social factors. Instrumentation will include small weather stations to track temperature, relative humidity, solar radiation; tree sapflow sensors; and sensors for soil moisture, conductivity, and temperature as a function of depth. The data will be used to determine relations between urban microclimate (temperature and relative humidity) and natural components (soil moisture and tree evapotranspiration) as a function of diurnal and seasonal changes, and to potentially relate the results to socio-economic factors. This research can be used to assess the utility of models in simulating soil moisture and evapotranspiration, taking into consideration governing urban microclimates over days and seasons.

Title: **Effects of Partial Throughfall Exclusion on Soil Dynamics in Lowland Tropical Forests Across Rainfall and Soil Fertility Gradients**

Daniela F. Cusack[1,2*], Lee H. Dietterich[1], Emily Blackaby[1], Nicholas Bouskill[3], Stephany Chacon[3], Amanda L. Cordeiro[1], Karis McFarlane[4], S. Joseph Wright[2]

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Project Lead Principal Investigator (PI): Daniela F. Cusack

BER Program: ESS

Project: Early Career project

Project Website: https://www.facebook.com/PARCHEDpanama/?modal=admin_todo_tour

Project Abstract (400 word):

Humid tropical forests contain some of the largest soil organic carbon (C) stocks on Earth. Despite the importance of C storage in this biome, controls over variation in soil C stock sizes and depth distribution remain poorly understood. We hypothesized that soil C dynamics and related ecosystem processes are more resistant to drying in lower rainfall and infertile sites, where plant and microbial communities are more adapted to stress. We used a partial throughfall exclusion established in 2018 in four Panamanian forests that span 2350 mm to 3300 mm mean annual rainfall, and variation in soil fertility. We measured soil C storage inputs, losses, microbial community characteristics, and nutrient availability. The experiment excludes ~50% of throughfall from plots using clear roofing over 10 *x* 10 m plots, diverting moisture out past 50 cm-deep plastic-lined trenches (n=4 per site, 32 plots total).

Across the four forests soil C dynamics vary with rainfall and soil fertility, and key processes responded to throughfall exclusion. First, soil respiration was lower in throughfall exclusion versus control plots, with interacting effects of site and season. This was similar to background patterns of decreased soil respiration during the natural dry season, with the magnitude of seasonal respiration shifts were predicted by soil moisture shifts and available phosphorus and base cations. Along with decreased soil respiration, the radiocarbon age of respired soil C was significantly

older in throughfall exclusion versus control plots. The decline in soil respiration could be related to reduced fine root (<2 cm diameter) production during, and/or to reduced microbial biomass, both of which appear to be declining with throughfall exclusion. For example, there was significantly less microbial biomass in throughfall exclusion versus control plots, including decreased fungal biomass. Also, microbial community composition changed with throughfall exclusion in infertile soils, converging toward a “drought microbiome”, whereby taxonomically similar bacteria were selected for by drying. At the same time, throughfall exclusion promoted accumulation of soil nitrogen during the dry season, and soil moisture data indicated reduced vertical flushing of soils during rainfall events in exclusion plots. These results suggest that drying in tropical forests is likely to alter soil C storage, although the net balance between reduced soil respiration, reduced root inputs, and changes in microbial processing remain to be seen. Continued research at these sites will be valuable for parameterizing and developing model processes to predict future C storage in tropical forests.

Title: Machine learning upscaling of land-atmosphere exchanges across North America to capture extreme impacts

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Project Lead Principal Investigator (PI):

BER Program: ESS – EESM

Project: DOE Early Career: Drought, heat and wildfire impacts on coastal water relations

Project Website: https://www.keenangroup.info/currentProjects.html

Project Abstract:

Eddy covariance networks have served as a primary tool to understand the dynamics of land-atmosphere interactions, in particular ecosystem-level photosynthesis (or gross primary production, GPP), ecosystem respiration, and water use. However, the eddy covariance technique provides only spatially sparse observations with limited representativeness. Thus, spatial upscaling of site-level measurements is often required to achieve regional and global synthesis. Here we explore novel machine learning frameworks informed by physical and physiological knowledge to upscale GPP from AmeriFlux eddy covariance network towards wall-to-wall maps over North America at 16-day and monthly temporal scales. Input datasets include remote sensing products from the Moderate Resolution Imaging Spectrometer (MODIS), satellite-based evapotranspiration, solar-induced chlorophyll fluorescence, and ERA5 atmospheric data. Models are trained with data from 2001 to 2017 and evaluated with spatiotemporal cross-validation as well as independent eddy covariance measurements after 2017 from National Ecological Observatory Network (NEON) sites. We find that incorporating physiological constraints improves machine learning models' ability to reconstruct interannual variability of land-atmosphere interactions by emphasizing extreme events which are often overlooked by standard learning algorithms due to their rarity. These improved estimates provide important insights into ecosystem-atmosphere feedbacks under a changing climate.

Soil production and chemical weathering rates along a vegetation gradient in the East River Watershed, Colorado

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Project Lead Principal Investigator (PI): Isaac J. Larsen

BER Program: SBR

Project: Early Career project

Project Abstract: Globally, mountain watersheds are hotspots for chemical weathering, but our process-level understanding regarding the mechanisms and drivers of chemical weathering in steep, high elevation landscapes is incomplete. To quantify the influence of vegetation on soil chemical weathering rates, soil samples were collected across a vegetation gradient on Mount Gothic, an igneous quartz monzonite intrusion in the East River watershed, near Crested Butte, Colorado. Three sampling sites are above tree line, at elevations >3700 m, whereas three additional sampling sites are at elevations <3400 m, where there is spruce forest vegetation. Bedrock samples were collected from outcrops adjacent to each of the soil pits to characterize the geochemistry of un-weathered parent material. The samples are currently undergoing analyses at the University of Massachusetts Cosmogenic Nuclide and XRF Laboratories. Though quartz-poor, the samples have yielded sufficient material for measurement of *in situ*-produced ^{10}Be, a cosmogenic nuclide that is used to assess rates of surface processes averaged over geomorphic timescales. The ^{10}Be concentrations will be used to quantify the total denudation rate, or the rate of mass loss due to the combined influences of physical erosion and chemical weathering (mineral dissolution). By measuring the enrichment of Zr, a chemically immobile element, and applying geochemical mass balance, the fraction of total denudation caused by chemical weathering will be quantified. The results will be used to determine rates of physical erosion and chemical weathering that will be used to assess the influence of vegetation on chemical weathering rates. Additional samples are to be collected at sites that span similar biotic and climatic gradients, but that have different underlying geology, which will further permit assessment of the factors that most strongly influence soil chemical weathering in the East River watershed.

Title: **Experimental Warming and Drying Increase the Age of Soil Respired Carbon and Alter Respiration Flux Rates in Lowland Tropical Forests in Panama**

Karis J. McFarlane[1]*, Daniela F. Cusack[2,4], Lee H. Dietterich[2], Alexandra Hedgpeth[1,3], Andrew T. Nottingham[4,5]

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Project Lead Principal Investigator (PI): Karis McFarlane

BER Program: ESS

Project: Early Career Project

Project Website:

Project Abstract: Tropical forests account for over 50% of the global terrestrial carbon sink and roughly one-third of global soil carbon, but the stability of carbon in these ecosystems under a changing climate is unknown. We assessed how a changing climate affects soil carbon stability in tropical forests, by using ^{14}C to determine the average age of soil respired carbon following experimental warming and drying. For two different *in situ* experiments - soil warming (via whole-profile heating by 4ºC) and soil drying (via partial throughfall exclusion) - we measured soil respired $^{14}CO_2$ for one year during the dry, dry-to-wet transition, and wet seasons. The background $\Delta^{14}C$ of soil respiration in these forests (16 ± 8 ‰ for control plots) reflected modern sources (<4 yr on average) and was 6 ‰ higher (one year older on average) during the dry-to-wet transition than later in the wet season. Experimental warming increased respiration rates and, during the wet season, increased the age of respired soil carbon by roughly 2–3 years ($\Delta^{14}C$ increased by 12 ‰ relative to controls). In contrast, experimental drying decreased respiration rates and increased the age of respired soil carbon by about 2 years ($\Delta^{14}C$ increased by 8 ‰ relative to controls). Together, these results indicate a relative shift in microbial carbon use towards older sources: warming by depleting the pool of rapidly cycling carbon and stimulating the decomposition of old carbon; drying by reducing the accessibility and subsequent decomposition of new carbon inputs. These findings imply a destabilization of old soil carbon under warming and a suppression of new carbon turnover under drying, which will have major implications for the tropical forest carbon cycle under climate change.

Title: Laboratory and Field Studies of Processes Impacting Reactive Nitrogen Oxide Fluxes to and from Soil

Authors: Jonathan D. Raff[1,2,3]*, Evan Z. Dalton[2], Adrien Gandolfo[1,3], Zachary C. Payne[2], Clara Lietzke[2], Rebecca Abney[1,3], Richard P. Phillips[4], Joanne E. Stubbs,[5] Peter J. Eng,[5] David Bish,[2] Lane Baker[2]

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Project Lead Principal Investigator (PI): Jonathan D. Raff

BER Program: ESS

Project: University project, Early Career project

Project Abstract:

Nitrogen (N) cycle processes play a crucial role in regulating the overall abundance of oxidized inorganic nitrogen in terrestrial ecosystems, and are responsible for initiating the subsequent loss of soil N via volatilization and leaching. This poster will outline our laboratory's effort to understand the sources and sinks of reactive nitrogen oxides (NO, NO_2, HONO) with the ultimate goal of improving how fluxes of reactive nitrogen oxides are represented in chemical-transport models. In this presentation we will share results of a field campaign carried out in 2021 that aimed at studying the emissions of reactive nitrogen oxides from soil and freshly senesced leaves in the autumn. We revealed that the leaves some deciduous tree species become sources of NO in forested regions when nitrogen that is not reabsorbed during senescence is released to the atmosphere. In addition, we will present results of a new study of the mechanism of HONO release from soil clay mineral surfaces at the molecular level. Specifically, the surface acidity of the kaolin mineral dickite was probed using scanning conductance ion microscopy (SICM) for the first time. Steps and edges consisting of incompletely coordinated aluminum hydroxide groups were found to be likely reactive sites that are responsible for the release of nitrite as HONO to the atmosphere at soil pH well above the pK_a of nitrous acid. Furthermore, we found that the basal planes of dickite exhibited a persistent negative charge, which was surprising given the anisotropic structure of dickite. To explore this observation we initiated a study of the structure of kaolin mineral surfaces and will present results on the first use of crystal truncation rod (CTR) diffraction to study kaolin mineral surfaces. These results open up a new realm of possibilities for studying reactions on clay mineral surfaces that impact atmosphere-soil exchange of atmospherically-relevant gases.

Impacts of Drying on Hyporheic Zone Biogeochemistry

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Project Lead Principal Investigator (PI): James Stegen
BER Program: Early Career Research Program
Project: Multi-watershed perturbation response traits derived from ecological theory

Project Abstract: All streams have zones that are under water sometimes and are dry at other times, most streams go fully dry, and the occurrence of dry streambeds is increasing. Within streams, hyporheic zones are often a primary biogeochemical reactor that influences carbon, nutrient, and contaminant transformations and fluxes. Arguably then, watershed and river corridor hydro-biogeochemistry research should have a high level of emphasis on studying hyporheic zones that are sometimes wet and sometimes dry (i.e., that are variably inundated). This is not the case, however, which means that we are understudying one of the most common stream habitats on the planet. This gap is increasingly recognized, and research efforts focused on variably inundated hyporheic zones are increasing. I will present one such study focused on the influences of drying on hyporheic zone biogeochemistry. The study has three primary goals evaluated in hyporheic zones distributed across the contiguous United States: (1) quantify the direction and magnitude of effect that drying has on aerobic respiration rate across diverse hyporheic zone environments, (2) reveal physical, chemical, and biologic mechanisms governing the impact of drying on respiration, and (3) incorporate that mechanistic knowledge into a reactive transport model aimed at predicting the influences of drying on variably inundated hyporheic zone hydro-biogeochemistry. Those goals are motivated by single-system experiments that found a negative impact of drying on respiration that was linked to a change in the chemistry of organic matter. That chemical change caused less energy to be available to microbes that use the organic matter for respiration. While those are interesting results, we don't know if similar results happen across other hyporheic zone systems. The current study is filling that gap and extending the outcomes to both data driven and mechanistic predictive models. Such knowledge and tools will help incorporate variably inundated hyporheic zones into our holistic understanding of Earth system hydro-biogeochemistry.

Understanding the Effects of Hydrometeorological Disturbances on River Water Temperature and Salinity at Regional to Continental Scales

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BER Program: ESS
Project: Early Career Project
Project Website: https://sites.google.com/lbl.gov/inaiads

The frequency, duration and intensity of hydrometeorological disturbances such as floods, droughts, and heatwaves are projected to increase with climate change, and can have drastic consequences to water quality in rivers. It is challenging to build generalizable models that analyze and predict how disturbances with variable spatial extent, timing and magnitude affect river water quality across catchments with different attributes . In this presentation, we describe results from a U.S. Department of Energy project iNAIADS that utilizes data-driven methods to understand water quality response and resilience to disturbances.

We examine the effects of heat waves on river water temperature and floods on salinity across basins with different climate, geological, land use and water management attributes using regional to continental-scale datasets. First, we present the use of classical machine learning and deep learning models to predict monthly and daily stream temperatures in the mid-Atlantic and Pacific Northwest regions for temporal predictions and spatiotemporal predictions in unmonitored basins (PUBS) that include pristine and human-impacted catchments. These models show that air temperature is the primary driver of stream temperature, and are used to inform how stream thermal regimes respond to heat waves. We discuss how the models account for the unpredictable timing, duration and spatial extent of extreme events by extrapolating information on water quality at regional scales from limited local observations, while accounting for its variations at both short and long timescales.

We then present an analysis of the response of river salinity (measured as specific conductance, SC), to floods across the continental US using statistical, machine learning and information theory approaches. Although dilution is the prevailing mechanism that regulates *SC* levels during floods, it is found that ~6% of flood events across all sites result in an increase of *SC* relative to the long-term mean. Our results also show that catchment aridity and anthropogenic impacts such as urbanization are primary factors resulting in distinct responses of salinity in rivers to floods. Moreover, we show that antecedent SC levels in the few days preceding the flood is the most dominant factor regulating the response of salinity to floods within individual sites.

We finally present the iNAIADS framework (iNtegration, Artificial Intelligence, Analytical Data Services) which comprises a data integration tool BASIN-3D that can be used to reproducibly synthesize diverse time-series data from distributed sources essential for such analysis, along with reusable analytical and machine learning codes for water quality modeling.

Title: Quantitative, Trait-Based Microbial Ecology to Accurately Model the Impacts of Nitrogen Deposition on Soil Carbon Cycling in the Anthropocene

Edward Brzostek[1*] Ember Morrissey[1], Zachary Freedman[2], Chansotheary Dang[1], Nanette Raczka[1], Juan Piñeiro[1, 4], Christopher Walter[1], Steve Blazewicz[3], and Peter Weber3

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Project Lead Principle Investigator: Edward Brzostek
BER Program: ESS
Project: EPSCOR; University Award

Nitrogen (N) deposition has enhanced carbon (C) storage in temperate forest soils. However, it remains unclear whether this soil C will persist as N deposition declines across the region. At the heart of this knowledge gap is the failure to link N-induced shifts in microbial biodiversity with traits that control microbes' ability to breakdown, assimilate or stabilize soil C. Given that this uncertainty directly impedes the ability of predictive models to project future soil C stocks, there is a critical need to determine how N-induced shifts in key microbial traits drive soil C stabilization. To address this uncertainty, our objectives are to: 1) Quantify variations in taxon-specific and community-level microbial traits across gradients in microbial community composition, the distribution of ectomycorrhizal (ECM) and arbuscular mycorrhizal (AM) trees, and N availability and 2) Integrate these data into a novel predictive framework that enhances our ability to project the regional soil C consequences of N deposition in temperate forests. To meet our empirical objectives, we used a suite of quantitative stable isotope probing, metabolomics, and biogeochemical approaches. We continue to build off our findings that decomposition pathways in AM soils have greater flexibility in which microbes are the active decomposers and what they produce than those in ECM soils. To do this, we performed two experiments to examine how N availability and root exudates impact microbial diversity and function. Under elevated N availability, we found evidence for a reduction in functional evenness for both mycorrhizal types with a narrowing of the distribution of active taxa taking up C and N. There was also a negative relationship between respiration and functional diversity suggesting that communities with a higher functional diversity may use resources more efficiently. Under simulated root exudation, we found that microbes in ECM rhizospheres are more efficient at converting exudates into biomass than microbes in AM rhizospheres. We used these results to develop new microbial groups based on substrate preference in our plant-microbial interactions model, FUN-CORPSE. We challenged the model to reproduce results from our laboratory and field experiments and have found that elevated N induces emergent shifts in the dominance of microbes that consume dissolved organic carbon, primary plant material, or microbial necromass. Coupled together, our experimental and model results highlight the importance of integrating state-of-the-art data on microbial traits and function into models to improve predictions of temperate forest responses to global change.

Flow Hydrodynamics and Transport Characteristics in Presence of Permeable Biofilms

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Project Lead Principal Investigator (PI): Rishi Parashar

BER Program: ESS

Project: EPSCoR Project

Project Abstract:

Biofilm images of Paenibacillus 300A strain, obtained from two-dimensional micromodel experiments, formed the basis for studying spatial organization of biofilms in pore networks and evaluation of their impact on flow and conservative solute transport characteristics. The micromodels were designed with hexagonal packing of equal diameter grains to simulate a pore network environment with simple parabolic flow profiles. Biofilm images were processed to represent them as synthetic porous structures with locally varying physical properties. The inclusion of these microstructures causes higher degree of spatial correlation in the numerical model, and produces local velocities orders of magnitude slower than those found in the main channels (away from the biofilms) of the micromodel. This flow heterogeneity leads to enhanced solute spreading in the breakthrough curves that exhibit extreme anomalous slopes at intermediate times and very marked late solute arrival times due to retention imparted by low velocity and stagnation zones. The efficiency of solute retention by the biofilms (i.e., trapping of solute particles within biofilm microstructures) is manifested in the long tailing of the breakthrough curves. The study shows that solute retention by biofilms exerts a strong control on conservative transport at the pore-scale, a role that has not received enough attention in the past. The integrated experimental and modeling approach is expected to serve as building blocks in understanding impact of biofilms for a broader range of pore geometries and flow conditions with implications for applications such as metal bioremediation.

Title: A Novel Halophyte-Capable Plant Hydraulics Model for Mangrove Forest Function

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Project Lead Principal Investigator (PI): Ashley M. Matheny

BER Program: ESS

Project: Exploring halophyte hydrodynamics and the role of vegetation traits on ecosystem response to disturbance at the terrestrial-aquatic interface (University Project)

Project Website: http://www.jsg.utexas.edu/matheny/halophyte-hydrodynamics/

Project Abstract: Mangroves grow along coastlines and intertidal zones, and are therefore very rarely limited by water availability. However, during the dry season, these ecosystems behave more similarly to semi-arid ecosystems than like well-watered forests. Mangroves likewise provide a critical carbon sink sequestering carbon at a rate disproportionate to ecosystem extents. Modeling the water and carbon dynamics of mangrove forests is a critical task for developing robust models of coastal climate processes, particularly in the face of sea-level rise and disruptions to local hydroclimates and therefore freshwater inputs.

Here, we present the development of a salt-exclusion water uptake module for the FETCH2 advanced vegetation hydrodynamics model that is capable of mechanistically simulating root osmoregulation by halophytes. FETCH2 approximates water flow through xylem as flow through non-saturated porous media and accounts for dynamic changes to conductance and capacitance of plant tissues caused by changes in water content. The FETCH2-osmo model bases vegetation water potentials on total matric, gravitational, and osmotic potentials at each height increment. Parameter sets within FETCH2 are based on measurable hydraulic properties. Studies have shown that many such traits can be highly plastic and vary spatiotemporally. Here, we use the findings of an on-going greenhouse-based study of mangrove hydraulic traits and their variability to parameterize our halophyte-capable version of FETCH2. These plant traits are complemented by environmental forcing observations from 4 field study sites are positioned to promote analysis of mangrove forest function across both humidity and salinity gradients which are predicted to change in response to disturbances such as sea level rise, precipitation variability, inundation frequency, and increased atmospheric CO_2. Within the greenhouse, we are able to test for species and population-level differences in adaptation and acclimation of different hydraulic traits to fluctuating humidity and salinity environments. This project supports mangrove monitoring in four sites across the globe: from humid (Panama) to arid (Abu Dhabi) and at the northern (Texas) and southern (Victoria, Australia) growth limits. Ultimately, the new FETCH2-osmo model with will integrate into the DOE's functionally assembled terrestrial simulator (FATES) within E3SM.

Title: **Droughts and Deluges in Semi-Arid Grassland Ecosystems: Implications of Co-occurring Extremes for C Cycling**

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Project Lead Principal Investigator (PI): Melinda D. Smith

BER Program: ESS

Project: University Project

Project Abstract:

Intensification of the global hydrological cycle is increasing the frequency of extreme climate perturbations including multi-year droughts and deluges (persistent, torrential rain events). Such climate extremes are known to have substantial impacts on ecosystem structure and function, but when these co-occur as compound climate extremes, their impacts are expected to exceed their independent effects. The overall goal of our proposed research is to assess how co-occurring drought and deluge climate extremes will impact key C cycling processes known to be important for carbon-climate feedbacks. We will address this goal via research in the 280,000 km^2 semi-arid shortgrass steppe ecoregion located at the western edge of the US Great Plains. Our research project will test the hypothesis that when a compound climate perturbation of an extreme deluge occurring within the backdrop of extreme drought, a combination of conditions converge (e.g., warm temperatures, abundant soil moisture, and increased soil N availability) to strongly stimulate C cycle processes, potentially resulting in "hot moments" or landscape-level "hot spots" (i.e., increases in biogeochemical processes in time or space that far exceed background levels). To test this hypothesis, we will conduct a field experiment designed to quantify the magnitude of C cycling responses to drought and deluge events (independently and combined) and identify the underlying mechanisms resulting in positive drought-deluge interactions that can lead to hot moments of C cycling. Both above- and belowground C cycle responses to climate extremes will be quantified during this 3-yr experiment. To scale-up from the plot-level experiment to the shortgrass steppe ecoregion, we will use historical climate data to quantify the regional frequency of potential drought-deluge interactions and remote sensing products to estimate C cycling sensitivity to droughts, deluges and their combined effects and to identify hot spots in C cycling regionally. Concurrent with these research activities, we will simulate extreme drought, deluge and drought-deluge perturbations with DOE's E3SM Land Model (ELM). We will explicitly compare the experimental results and remotely

sensed observations of drought-deluge compound climate perturbations to ELM simulations, with the expectation that the process-level understanding gained from our field experiment and remote sensing analyses can be used to constrain process representation and parameterization in ELM, and to improve Earth System projections of ecosystem C-cycling responses to droughts and deluges at the ecoregion scale.

Title: **Instream and Hyporheic Zone Contributions to River Corridor Oxygen and CO_2 Dynamics During Particulate Organic Matter Additions**

Anna B. Turețcaia[1], Bing Li[2], Philip C. Bennett[1], Matthew H. Kaufman[3], Xingyuan Chen[3], Xiaofeng Liu[2], James Stegen[3], and M. Bayani Cardenas[1,*]

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Project Lead Principal Investigator (PI): M. Bayani Cardenas

BER Program: ESS

Project: Respiration in hyporheic zones: connecting mechanics, microbial biogeochemistry, and models (DE-SC0018042; University Project)

Project Abstract:

River corridors are important for aquatic and terrestrial nutrient and organic matter (OM) cycles. Thus, there have been numerous studies to understand the role of the river channel versus the benthic sediment in OM transformations. Yet gaps remain regarding when and where reaction hot spots occur within the river corridor's terrestrial-aquatic interface. Here, we combined experimental and modeling approaches to evaluate the contributions from the channel and from the most biogeochemically active portion of the river sediment – the hyporheic zone– to the aerobic respiration of additional OM. We conducted flume experiments where we intermittently added different masses of OM to the channel. Through monitoring aerobic respiration and other parameters in both the channel and the hyporheic zone, and through robust determination of mass transfer coefficients, we developed a two-box dynamical model representing the hyporheic zone-channel-atmosphere system. We found that under the low channel flow conditions of the experiments and on hourly-to-daily timescales: (1) the aerobic respiration of OM mostly occurs in the channel; (2) the CO_2 concentration in the hyporheic zone always exceeds the CO_2 concentration in the channel, but due to weak hyporheic zone-channel coupling, the hyporheic zone is a small contributor to aerobic respiration of the entire river corridor; (3) the channel-atmosphere exchange flux exceeds the hyporheic zone-channel flux by orders of magnitude; (4) and, the modeled channel CO_2 levels agree markedly better with the observations when the respiratory quotient is 0.5 instead of 1. Thus, under our experimental conditions, the addition of OM resulted in the channel acting as the river corridor's hot spot for aerobic respiration although aerobic respiration was always active in the hyporheic zone.

Title: Root Dynamics and Ecosystem Legacy, Exploring Responses and Dynamics at Three Midwestern United States AmeriFlux Sites

Benjamin J Ahlswede[1], Beth Drewniak[2], Miquel Gonzales-Meler [2], Max Berkelhammer[1]

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Project Lead Principal Investigator (PI): Max Berkelhammer

BER Program: [ESS]

Project: Water foraging with dynamic roots in E3SM; the role of roots in terrestrial ecosystem memory on intermediate timescales

Project Website: NA

Project Abstract:

The effects of stress events, such as drought or heatwave, on forest ecosystems typically persist for months or years after the initial event itself, a phenomenon often referred to as legacy. As extreme events increase in frequency and duration, the compounding effects associated with extended legacy may influence how forests will respond to climatic change. Forests respond to stress by allocating resources to where they are most needed, by redistributing fine roots deeper into the soil during times of drought. These belowground changes may ameliorate stress in the short term while also leading to long term costs and therefore protracting the response to the initial event. These expected changes to root systems in response to stress, and other dynamics that lead to legacy are not present in modern Earth System Models, reducing our ability to predict ecosystem responses to stress. Here, we utilize the Exascale Earth Systme Model (E3SM) in conjunction with a dynamic root module - where plants can forage for water and nitrogen - to understand how root systems respond to stress and how these changes influence legacy. Firstly we, examined the role of legacy globally, with and without root dynamics. We found that by allowing roots to forage, the timetable of recovery from stress events is altered differentially between dry and humid ecosystems. We then use point scale simulations in three forest flux sites in the Midwest, Morgan Monroe State Forest (US-MMS), Missouri Ozarks (US-MOz), and Sylvania Wildernsess (US-Syv), where eddy covariance tightly constrains carbon and water fluxes. We conducted a sensitivity analysis at these three sites, using an ensemble of simulations assessing the response to root longevity and fine root to leaf allocation. We then partition the sources of legacy in these systems between long term responses to weather events, and implicit legacy related to the land-use and biological history. Future

work will compare these modeling results with tree ring observations from these sites and linking E3SM to a dynamic allocation module. These analyses improve our understanding of legacy effects and forest response to stress, creating opportunities for improved predictive and mechanistic understanding of future conditions.

Notes on abstract:

- Please Bold the Abstract title
- Note the placement of superscripts in the authors and affiliations.
- Please use size 12 Times New Roman font
- URL above should be specific to the project. More than one URL is permitted.
- **References**, if necessary, can be **Publications** instead, if needed. Use any common style for these citations.
- For combined Lab submissions (e.g., SFA's or NGEE), please submit the abstracts in the order that you would like to have the abstracts and posters presented (i.e., the overview poster abstract first).
- Do not include any Personally Identifiable Information (PII) or confidential information (e.g., SSN#, pending patents, etc.) since abstracts will be publicly posted online.
- If you have questions, please contact Aaron Grade (Aaron.Grade@science.doe.gov) or Brian Benscoter (Brian.Benscoter@science.doe.gov).

Title: Linking root and soil microbial stress metabolism to watershed biogeochemistry under rapid, year-round environmental change

Jennifer M. Bhatnagar,[1]* Michael Silverstein[1], Kristen DeAngelis,[2] Charles Driscoll,[3] Caitlin Hicks Pries,[4] and Pamela H. Templer[1]

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Project Lead Principal Investigator (PI): Jennifer Bhatnagar

BER Program: ESS

Project: Linking root and soil microbial stress metabolism to watershed biogeochemistry under rapid, year-round environmental change

Project Website: https://people.bu.edu/ptempler/workDetails/climateChangeWinter.html

Project Abstract:

Air temperatures are rising, while the winter snowpack is shrinking and soil freeze/thaw events are increasing in high latitude ecosystems. The severe thermal impact of soil freeze/thaw cycles in winter, coupled with warming during the growing season, reduces soil carbon (C) cycling, but increases nitrogen (N) and phosphorus (P) cycling in soil. Nevertheless, the root and microbial mechanisms leading to these shifts are unclear. We hypothesise that under climate change across seasons, microbes and plants exhibit a trade-off between stress metabolism and soil C, N, and P uptake (short term) and biomass stabilization (longer term) that scales up to impact C and nutrient export at the watershed-level. To test this hypothesis, we are conducting a model-data integration study using the Climate Change Across Seasons Experiment (CCASE) at the Hubbard Brook Experimental Forest (HBEF) and a plot-to-watershed-level biogeochemistry model, PnET-BGC. At CCASE, replicate field plots receive one of three climate treatments: growing season warming (+5˚C above ambient), warming + freeze/thaw cycles (+5˚C above ambient in growing season plus up to four freeze/thaw cycles in winter), and reference conditions (no treatment). We have found that warming + freeze/thaw cycles induces redox stress that selects for anaerobic N cycling-microbes, while potentially shifting the majority of microbial C-cycling activity from organic to deeper mineral soil horizons during winter. Soil microbes are also evolving under these conditions to increase decomposition of plant and soil C, but decrease decomposition of organic P, potentially decoupling C, N, and P outputs to associated aquatic ecosystems both temporally and spatially. Ongoing research couples new belowground biogeochemistry measurements at CCASE in organic and mineral soil horizons with soil metagenomic data and new high-throughput characterizations of trait and gene evolution in individual soil bacteria and fungi to reconstruct evolution of potential plant and microbial C, N, and P metabolism at CCASE over the past decade. We will incorporate

immediate and evolved responses of microbial C, N, and P cycling into new versions of PnET-BGC, including an evolutionary algorithm applied to specific C, N and P flux calculations. This research tesst our conceptual understanding of plant and microbial physiology responses to severe, compounding soil temperature perturbations across seasons, as well as the utility of a forest stand-level manipulative climate change experiment to understand the biogeochemical dynamics of a forest watershed undergoing rapid environmental change.

Title: **Snow pattern evolution in the East River SFA simulated with a distributed snow model and Airborne Snow Observatory data**

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Project Lead Principal Investigator (PI): Jeffrey S. Deems

BER Program: SBR

Project: University project

Project Abstract:

Spatial and temporal patterns of snow accumulation and melt dominate hydrologic and biogeochemical flows in temperate mountain catchments. Mountain snowpack states, fluxes, and properties exhibit extreme and scale-dependent variability, complicating efficient sampling and modeling. Evaluating system perturbation impacts on water availability and nutrient cycling depend on robust observations and simulations of seasonal snow dynamics at appropriate scales.

To explore snow accumulation and melt process dynamics over meter to watershed scales, we implemented a physically-based snow cover evolution model (Liston et al., 2006) at multiple grid resolutions, using combinations of accumulation process sub-models.

Model wind transport parameters were optimized in Senator Beck Basin, a well-instrumented nearby study site, and transferred to the East River SFA where instrumentation is less reliable.

To improve model results and system disturbances impacts analysis, we:

(i) implement and validate the albedo decay parametrization from Deems et al., 2013.
(ii) define a new forest type to allow wind sheltering of adjacent areas
(iii) explore precipitation assimilation and validation methods via in-situ and Airborne Snow Observatory measurements of snow depth and water equivalent (SWE), using both HRRR and WRF model forcings

These results help characterize the snow hydrologic system in the East River and assess the importance of snow distribution due to wind and gravitational transport at the watershed scale, providing the foundation for our ongoing long term system perturbation work and for integration with simulations of connected systems within the SFA.

References:

Liston, G.E., Elder, K., 2006. A Distributed Snow-Evolution Modeling System (SnowModel). *J. Hydromet*. 7, 1259–1276.

Deems, J. S., et al. 2013. Combined impacts of current and future dust deposition and regional warming on Colorado River Basin snow dynamics and hydrology. *Hydrol. Earth. Sys. Sci.* 17(11): 4,401-4,413.

Ecohydrological Controls on Root and Microbial Respiration in the East River Watershed of Colorado

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Project Lead Principal Investigator (PI): Mariah Carbone
BER Program: ESS
Project: University Project
Project Website: https://carbone-lab.nau.edu/index.php/snodgrass-mountain-transect/

Belowground in the soil, microbes breakdown organic matter, releasing CO_2. Plant roots produce CO_2 also, via their metabolism. Our research seeks to understand how moisture inputs, such as snow and rain, influence the amount of CO_2 produced belowground in the East River watershed, near Crested Butte, Colorado. In June 2021 (Year 1), we instrumented four sites along Snodgrass Mountain in the two main forest types, aspen and spruce/fir to quantify the flux of CO_2 from the soil to the atmosphere, and how plant and microbial sources of CO_2 respond to the environment, across different elevations. To do this, continuous measurements of soil CO_2 concentrations, at multiple depths, will be combined with novel radiocarbon (^{14}C) methods (Year 2) that will enable the separation of plant and microbial sources of CO_2. These measurements will be linked to measurements of forest and snow phenology (with PhenoCams), microbial activity, tree growth and water status, and environmental factors such as air and soil temperature, soil moisture, and groundwater table. Our work is motivated by our overarching hypothesis that quantifying belowground plant and microbial processes separately, and how they are influenced by snow and rain inputs, is necessary for understanding and predicting how the belowground East River watershed ecosystems will respond to changes in the environment.

To date, continuous 30-minute records from all deployed sensors have been logged at each site and transmitted remotely via cell modem to NAU. This initial snow-free season of data (June 2021 through October 2021) shows interesting forest type and seasonal patterns of soil CO_2 fluxes. Across the gradient, mid-elevation forests had much larger seasonal soil CO_2 fluxes (aspen=309, conifer=474 g C m^2) compared to high-elevation conifer and low-elevation aspen forests, 166 and 124 g C m^2, respectively. Fluxes peaked in August and September across forests and elevations coinciding with the warmest soil and air temperatures and driest soil moisture. Aspen forest CO_2 fluxes strongly declined in October coinciding with PhenoCam derived canopy greenness and leaf-fall. We are currently planning and preparing for field measurements for Summer 2022, where we will install new automated point dendrometers to measure tree growth, soil surface collars for manual CO_2 flux measurements, and collect ^{14}C samples to separate of plant and microbial sources of CO_2.

"Sticky Roots" – Rhizodeposition and the fate of mineral-associated soil carbon

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Project Lead Principal Investigator (PI): Zoe Cardon
BER Program: ESS
Project: University project

Mineral-associated organic matter (MAOM) is a dominant component of total soil carbon. Once bound to reactive soil minerals, that organic matter can be protected for millennia. In previous lab experiments, however, we have shown that individual compounds commonly released by roots can mobilize MAOM off minerals via direct and indirect mechanisms, making it vulnerable to microbial attack. We are exploring the mechanisms underlying root-induced mobilization of MAOM, and the longer-term, larger-scale implications of that mobilization.

Experimentation: We have developed a tool to manipulate rhizodeposition: controlled viral infection of plants. Barley Yellow Dwarf Virus (BYDV) attacks a broad range of grasses and increases phloem flow, potentially spurring increased delivery of phloem contents to the rhizosphere. We are testing effects of that virus-altered rhizosphere chemistry on MAOM mobilization by exposing plants (*Avena sativa*) to aphids, some carrying BYDV, and some not. **(Result 1)** When infected and uninfected plants were grown from a young age in nutrient replete conditions hydroponically, the solutes in hydroponic liquid around infected vs. uninfected roots differed (as assayed by FTICR-MS). When those solutes were added to nonsterile soil laced with ferrihydrite loaded with ^{13}C-glucose (as a surrogate for MAOM), ~75% more MAOM mobilization and mineralization (as evidenced by $^{13}CO_2$ release) was driven per unit root biomass by solutes gathered around infected plant roots. **(Result 2)** When oats were grown hydroponically to large size, then half were infected with BYDV, virus-infected plants exhibited slightly reduced median leaf number ~10 days after infection. By ~2.5 weeks, virus infection drove ~20% *increase* in DOC in hydroponic solution around roots of infected plants, despite the reduced median leaf number. **(Result 3)** When young BYDV-infected and uninfected oats were grown in soil, plant biomass, photosynthetic rates, and root:shoot ratios were reduced by infection. Amplicon sequencing revealed infection-linked alteration of microbial community composition. **(Activity 4)** We are now conducting a capstone greenhouse soil experiment using BYDV-infected and uninfected *Avena*, testing two hypotheses: Viral infection will intensify ^{13}C-MAOM mobilization and mineralization at root surfaces in soil, but reduced root biomass in infected plants may result in a reduction of whole soil column mineralization of ^{13}C-MAOM.

Modeling: Using *ecosys*, we will test the hypothesis that root-induced MAOM mobilization and mineralization, resulting in entrainment of nutrients (N and P) into actively cycling pools, drives a positive feedback spurring enhanced plant productivity, rhizodeposition, and soil carbon storage in the longer term.

Trace Metal Dynamics and Limitations on Biogeochemical Cycling in Wetland Soils and Hyporheic Zones

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Project Lead Principle Investigator (PI): Jeffrey G. Catalano

BER Program: SBR

Project: University Award

Project Abstract:

Biogeochemical cycling in subsurface aquatic systems is driven by anaerobic microbial processes that employ metalloenzymes. Pure culture studies reveal that low availability of trace metals may inhibit methanogenesis, mercury methylation, and reduction of N_2O to N_2 during denitrification. However, whether such limitations occur in natural subsurface aquatic systems is currently unclear. This project seeks to establish mechanistic links between trace metal availability and biogeochemical transformations in subsurface systems. Integrated field and laboratory studies of trace metal availability and biogeochemical processes were conducted in riparian wetlands in the Tims Branch watershed at the Savannah River Site, marsh wetlands at Argonne National Laboratory, and the streambed of East Fork Poplar Creek at Oak Ridge National Laboratory. The speciation of trace metals in wetland soils and stream sediments shows surprising consistency across the field sites. Dissolved metals also show consistent uptake behavior by the soils and sediments but form distinct species at each site. Geochemical controls on trace metal availability may thus be site-specific despite similar native solid-phase speciation and binding affinities. Maximum bioavailable concentrations of ~10 nM for Cu and ~40 nM for Ni and Co occur in the porewater of stream sediments, below optimal for biogeochemical processes. The addition of Cu stimulates N_2O reduction in stream sediments and riparian wetland soils but not in marsh wetland soils. Production of CH_4 in riparian wetland soils increases by 75% following addition of Ni but marsh wetland soils generate indistinguishable amounts of CH_4 after similar amendment. Metal limitations on biogeochemical processes thus vary in occurrence among subsurface aquatic systems despite low metal availability across sites. Redox fluctuations in wetland soils and stream sediments promote Co and Zn availability and inhibit Cu availability under anoxic conditions. Oxic conditions in stream sediments and anoxic conditions in riparian wetland soils increase Ni availability. Repeated cycling of redox conditions enhance Zn and Cu bioavailability but decrease Ni and Co bioavailability. Metal limitations on biogeochemical processes may thus differ between consistently anoxic systems and those that redox cycle.

Title: **Tropical Rain Forests, Drought, Hurricanes and Heat: Results from the TRACE Experiment to Date**

Molly A. Cavaleri,[1]* Sasha C. Reed,[2] Tana E. Wood,[3] Benedicte Bachelot,[4] Aura M. Alonso-Rodríguez,[5] Kelsey R. Carter,[6] Daniela Yaffar,[7,8] Robert P. Tunison[1]

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Project Lead Principal Investigator (PI): Molly A. Cavaleri

BER Program: ESS

Project: University Project: "Interactive effects of press and pulse disturbances on biogeochemical cycling of a wet tropical forest in Puerto Rico"

Project Website: https://www.forestwarming.org/

Project Abstract:

Global climate change has led to rising temperatures and more frequent and intense climatic events, such as storms and droughts. These changes may have non-additive effects on ecosystem processes, resulting in complicated legacies we have yet to understand. We will present recent results from the Tropical Responses to Altered Climate Experiment (TRACE) in Puerto Rico, which was exposed to a severe drought, two years of experimental warming, and two major hurricanes, to assess the resilience of tropical forests to multiple disturbances. Plant community composition has been resistant to change (drought, warming, hurricane) over the timescale of this study. With warming, seedling survival increased with increasing density of the same species. These positive density-dependent feedbacks may lead to declined diversity with continued warming. Photosynthesis at optimal temperatures decreased in the experimental warming plots for understory shrubs, and there was no apparent thermal acclimation of optimum temperatures. One of the species did acclimate to warmer temperatures by expanding the thermal photosynthetic niche. Relative survival of both understory shrubs correlated with their ability to physiologically acclimate to warmer temperatures. Root production and standing stock was reduced in response to warming. This response was exacerbated following hurricane disturbance, such that prior warming led to significantly reduced root recovery. Root specific respiration was not influenced by warming or hurricane disturbance, yet root respiration rates were positively correlated with root nitrogen. We have seen relatively little physiological acclimation of the

understory vegetation to warmer temperatures for root processes, whereas aboveground physiological acclimation was species-dependent. While the community composition was resistant to change, should warmer temperatures continue, it is likely that a shift in community composition could occur. Total soil respiration rates were significantly higher in warmed plots, which appeared to be driven by microbial and not root responses. The temperature sensitivity (i.e., Q_{10}), however, was ~50% lower in warmed plots, suggesting a mechanistic shift. Even with reduced Q_{10}, if observed soil respiration rates persist in a warmer world, the feedback to future climate could be considerably greater than previously believed.

Title: Microbial contributions to environmental iron oxidation at the Savannah River Site

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Project Lead Principal Investigator (PI): Clara Chan
BER Program: ESS
Project: University Project

Project Abstract:

At the Savannah River Site (SRS) in South Carolina, extensive iron-oxidizing microbial mats form and appear to be a major sink of uranium. To understand the significance of microbial Fe oxidation and incorporate it into hydrobiogeochemical models, we need to know the environmental rates of biotic and abiotic oxidation, and the controls on these rates. To evaluate this, we conducted two field campaigns to the SRS to sample iron mats at two sites in the Tim's Branch stream and wetlands. We performed iron oxidation kinetics experiments on these terrestrial freshwater iron mats, in conjunction with 16S rRNA gene sequencing and metagenomic analyses of mats to identify the major iron oxidizing bacteria (FeOB) and the flanking community. The iron mats were dominated by known FeOB, notably a diverse set of *Gallionella* OTUs. We compare biotic oxidation rates with abiotic azide-killed controls and show that mat iron oxidation is dominated by biotic oxidation while oxidation by killed mat was much slower (2-9% of total rate in dark incubations). There was also relatively low oxidation in filtered controls in light and dark treatments (3-6% of total rate). Scanning electron microscopy shows the major morphologies in the mats are FeOB biominerals, including twisted stalks and sheaths. We have enriched a stalk-forming *Gallionella* (>97% of culture) from the wetland iron mats, and are continuing to isolate for further metabolic and genomic analyses. This work is part of a larger project focused on integrated kinetics, 'omics, and metabolic modeling work. We will present the results of metagenomic sequencing of the Fe mat communities used in the kinetics experiments, including the major physiological mechanisms of the dominant FeOB. These results set the stage for metatranscriptomics analyses and microbial modeling work towards our longer-term goal to link FeOB metabolic models and kinetics to biogeochemical models in order to predict Fe, C, nutrient and contaminant metal cycling.

Title: How does mercury methylation respond to intensive forest management and the creation of anoxia in floodplain soils?

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BER Program: ESS

Project: University project

Project Website: N/A

Project Abstract:
It is well known that silvicultural practices such as clear-cutting and thinning would alter productivity and hydrology of forest watersheds, which may also mediate a mercury (Hg) cycling response involving methylmercury (MeHg) production. In this study, we are conducting a field study with three transects covering the upland, midland riparian, and wetlands within thinned, clearcut and uncut control areas within a first-order watershed in the lower Atlantic coastal plain on the Santee Experimental Forest in South Carolina, USA. Each transect is instrumented to monitor soil moisture, temperature, redox, water table depth, and insolation. Commencing July 2021, we collected monthly composite soil samples (0-10 cm) at each site. From the initial data in July and August 2021, we found that the soil organic matter content increased significantly from upland (7.46 %) and midland (9.37 %) to lowland (18.55 %) ($p<0.05$). Due to the intimate association of Hg with soil organic matter, total Hg content followed this trend, i.e., upland (35.00 ng/g) and midland (48.49 ng/g), to lowland (75.14 ng/g) ($p<0.05$). We also observed a similar spatial trend of toxic MeHg, i.e., upland (0.34 ng/g) and midland (0.35 ng/g), to lowland (0.50 ng/g) ($p<0.05$). When we compared MeHg levels across treatments at the same spatial position of the transect, we found that soils had much significantly higher MeHg in both harvest (0.75-0.77 ng/g) and thinning (0.66-0.70 ng/g) treatments in both upland and midland than the control upland and midland (0.34-0.37 ng/g) ($p<0.05$), but we found the opposite results for the lowland wetland site (i.e., 1.59 ng/g for control, 0.79 ng/g for harvest, and 1.32 ng/g for thinning). Additional field sampling through September 2022 will help affirm these spatial differences, if any

Predicting hot spots and hot moments of biogenic gas accumulation and release in a subtropical ecosystem using airborne ground-penetrating radar (GPR)

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BER Program: ESS

Project: University project,

Project Website: not applicable

Project Abstract: [Limit to 400 words, size 12 Times New Roman font characters]

Peat soils are major terrestrial carbon stores and large natural producers of biogenic greenhouse gases (e.g., methane and carbon dioxide). These gases accumulate in the soil matrix to be subsequently released to the atmosphere, therefore directly influencing climate change. While recent advances have been made with regards to the prediction of carbon fluxes, many uncertainties still exist to properly understand the spatial distribution of hot spots and hot moments for the accumulation and release of biogenic gases. This can be attributed to the limitations in terms of effective non-invasive methods that can be deployed at scales of measurement relevant for the imaging and identification of such hot spots. This project intends to test a prototype ground-penetrating radar (GPR) unit mounted on a small unoccupied aircraft system (sUAS) to efficiently identify the presence of hot spots and hot moments in subtropical peat soils of the Everglades and explore how certain physical (i.e. soil structure) and biochemical properties (i.e. metabolic pathway) may influence its dynamics. As a preliminary phase, a series of measurements both at the laboratory and field scales were performed to test the ability of GPR to identify contrasts in relative dielectric permittivity associated with variable soil biogenic gas content for different antenna ground couplings (i.e. variable air gaps). Measurements were performed in soils from the Grassy Waters Preserve, a 60 square km wetland ecosystem near West Palm Beach (FL) that represents a pristine remnant of the historical Greater Everglades system. At the laboratory scale, a high frequency antenna was suspended over a peat monolith (extracted from the same site) using a custom-made rail system that allowed for the antenna to move autonomously and monitor changes in dielectric permittivity associated with biogenic gas build up and release at high temporal resolution. At the field scale, an array of antennas (with

frequencies ranging from 160-750 MHz) suspended from a wooden frame were also tested to determine the antenna frequency with the best compromise between resolution and depth of penetration when targeting hot spots for gas accumulation. Preliminary results are consistent at showing the potential of GPR for efficiently imaging hot spots for gas accumulation in a variety of settings, and therefore show promise for expanding scales of measurement via airborne/drone GPR.

Title: **Using Mercury Stable Isotopes to Identify Sources of Methylmercury to Aquatic Food Webs.**

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BER Program: ESS
Project: University-Led Research
Project Website: n/a

Project Abstract:

Historical and ongoing releases of mercury (Hg) have resulted in a legacy of Hg contamination in streambed sediment, streambanks, and floodplain soils downstream of the Y-12 National Security Complex (Y12), along the flow path of East Fork Poplar Creek (EFPC) near Oak Ridge, Tennessee. Elevated concentrations of inorganic mercury within this ecosystem have been shown to be associated with elevated concentrations of methylmercury (MeHg) in biota, including benthic invertebrates and fish. However, determining the specific ecosystem source(s) of MeHg that are being contributed to the food web can be challenging. Mercury stable isotope analysis is a powerful tool that allows us to trace biogeochemical pathways and track the transport and fate of sources through complex ecosystems. During previous studies, we have compared measurements of the total mercury isotopic composition of fish in EFPC and the Hinds Creek reference site, and have attempted to use linear regression techniques that utilize the varying percentage of MeHg content (i.e., %MeHg) among organisms to estimate the isotopic composition of MeHg sources within the ecosystem. While this indirect approach succeeded within the reference site, linear regression could not be utilized to estimate the isotopic composition of MeHg within the point-source-contaminated EFPC. Thus, the final objective of our broader ongoing proposed research was to develop a method to directly quantify the MeHg isotopic composition within EFPC biota, which are natural accumulators of MeHg being contributed to the EFPC ecosystem. Here, we successfully developed a novel method for the extraction, isolation, and direct determination of the compound-specific mercury isotopic signature of MeHg in biota. Application of this new method showed that: (i) the isotopic composition of MeHg accumulating in biota was distinct in the upper and lower reaches of EFPC, as well as differing from the reference site; (ii) the isotopic composition of MeHg within the reference site was clearly influenced by precipitation sources, while MeHg accumulating within EFPC biota was not; and (iii) the photochemical processing of MeHg sources within point-source-contaminated watersheds (i.e., EFPC) may differ from those influenced primarily by atmospheric deposition. Overall, these new methods that allow for direct measurement of compound-specific MeHg isotope composition will likely continue to lead to new insights that would otherwise be masked by the assessment of total mercury isotopic composition alone.

Title: **Deciphering Controls on Nutrient and Contaminant Migration Within Floodplains: The Critical Role of Redox Environments and Hydrologic Extremes**

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BER Program: ESS

Project: University Project

Project Abstract:

The fate and transport of nutrients and contaminants in soils and sediments are controlled by a complex network of biogeochemical reactions coupled with hydrologic processes. A major control on metal mobility in surface and subsurface systems is exerted by natural organic matter (DOM), albeit one that is poorly understood. Divergent OM transformation pathways drive variation in the chemical composition of DOM across watersheds. Yet, how this variation influences the functional composition and metal binding properties of DOM remains largely unexplored. Further, the source and impact of hydrologic extremes on biogeochemical processes and resulting fate and transport of nutrients and contaminants need to be assessed.

Our project elucidates the effect of redox conditions resulting from differing hydrologic regimes on formation and transport of soluble metal-organic complexes, and we explore the impact of varying sources of hydrologic extremes on nutrient-contaminant fate and transport. We use a combination of field measurements and laboratory experiments to examine the relationships between redox conditions, functionality of dissolved organic matter, and metal speciation (specifically examining metal-ligand complexes). Floodplain biogeochemical variation through climatic extremes and beaver-induced hydrologic variation at East River provide a unique look at controls on nutrient-contaminant fate and transport. Through our work, we have developed a novel approach that provides an unprecedented ability to resolve aqueous metal-organic complexes that reveals metal binding preferences for NOM based on metal-ligand chemistry. Importantly, we show that beaver dams have an outsized influence on hydrologic extremes, dwarfing the impact of climatic variation, that ultimate control biogeochemical conditions and water quality. Ultimately, our work is helping to advancing a robust predictive understanding of how hydrologic changes in watersheds affect water quality and inorganic element/contaminant loading.

Title: Sap Flux-scaled Transpiration, Canopy Conductance and Gross Primary Productivity in Response to Throughfall Manipulation in Three Co-occurring Species

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Project Lead Principal Investigator (PI): Jeffrey Dukes

BER Program: ESS

Project: University project: Understanding spatial and temporal drivers of variation in tree hydraulic processes and their consequences for climate feedbacks

Project Abstract: We recently started INATWE, the INdiana Acclimation of Trees to Water stress Experiment, in three forests in Indiana. This project will examine whether long-term exposure to different levels of water availability alters trees' short-term responses to droughts, and integrate results from the project into the FATES-HYDRO model and other models. It is still too early to present results from this project. Here, we present results from preliminary experiments conducted in deciduous forest in west-central Indiana. We investigated the influence of decreased precipitation and increased soil water limitation on (1) within- and across-season rates of transpiration, canopy conductance and gross primary productivity, (2) responses of these variables to soil moisture and other environmental conditions, and (3) responses to soil and atmospheric moisture during natural droughts. Using a 3-year throughfall exclusion experiment, we examined responses of co-occurring tree species to reduced water input and soil water availability by quantifying physiological responses for three deciduous species across ambient rainfall, moderate (-45%), and extreme (-80%) throughfall removal treatments. Our initial results from this ongoing research suggest that throughfall removal alters tree species' relationships between shallow soil moisture and transpiration, canopy conductance, and gross primary productivity. Trees in the drier treatments were frequently less responsive to fluctuations in soil moisture. These trees were also more physiologically conservative; at a given soil moisture level, these trees exhibited reduced transpiration, canopy conductance, and gross primary productivity compared to trees receiving ambient precipitation.

Methane Dynamics of Vegetation-Soil Interactions in Bald Cypress and Other Bottomland Hardwood Forests

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Project Lead Principal Investigator (PI): Bassil El Masri

BER Program: EES

Project: University project

Project Abstract

Methane (CH_4) is one of the most important greenhouses gas and more than 30% of the total CH_4 emissions originate from wetlands. There is high uncertainty in the contribution of mineral soil wetland to global CH_4 budgets. *Our project objectives are (1) to improve our understanding of the controls on CH_4 fluxes in forested mineral soil wetlands, and (2) to better understand the effects of landscape position and forest composition on the CH_4 fluxes between terrestrial ecosystems and the atmosphere*. *Using a coupled modeling-experimental approach*, we plan to measure the spatial and temporal dynamics of CH_4 fluxes in soils and woody structures (stems and "knees") of temperate bald cypress (*Taxodium distichum*) and other bottomland hardwood stands and incorporate our measurement into a land surface model to improve the model representation and predictions of CH4 fluxes. We are currently selecting suitable sites within the Clarks River National Wildlife Refuge (CRNWR) and Murphy's Pond in Western Kentucky that span a hydrologic gradient from the terrace to the stream channel. Soil's physical and chemical properties have already been measured at terrace sites. Preliminarily results show a significant difference in soil phosphorus loss and uptake by post oak and cherry bark sites and will be considered in future modeling efforts. Results from this project will enhance our understanding of CH_4 processes at bald cypress swamp and bottomland hardwood forests and will improve our knowledge of environmental processes in a hydrologically oscillating zone on CH_4 fluxes.

Peatland hydrology across scales: wintertime controls of spring water table and streamflow

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BER Program: TES

Project: Peatland hydrology across scale: a probabilistic framework for confronting variability, heterogeneity, and uncertainty (University award)

Our project aims to guide future representations of peatland hydrology and water-carbon feedbacks within Earth System Models, by improving process understanding and developing parsimonious models that elucidate the effects of hydroclimatic variability and spatial heterogeneity. Our research questions are centered on the three key drivers of peatland hydrology: (1) seasonal and interannual hydroclimatic fluctuations, (2) spatial heterogeneity of bog microtopography, and (3) hydrological connectivity across landscape units within a peatland watershed. Our analyses and model development use existing long-term datasets within the Marcell Experimental Forest (MEF), with new data collected whenever necessary.

To date, we have demonstrated the strong influence of water table elevations on the temperature sensitivity of CH_4 emissions, using a newly developed eddy covariance dataset spanning eleven years at MEF (Feng et al. 2020). Specifically, higher water tables dampen the springtime increases in CH_4 emissions as well as their subsequent decreases during the fall, resulting in hysteresis. These results imply that any hydroclimatological changes in peatlands that shift seasonal water availability from winter to summer will increase annual CH_4 emissions, even if temperature remains unchanged. To further investigate seasonal hydrological changes, we installed automated water table gauges across four bog-forest boundaries (the “lagg”) in two watersheds at MEF, which are hotspots of intense biogeochemical activity. These measurements will give us new information about the extent of lagg expansion and contraction during high intensity rainfall and snowmelt events.

Finally, we investigated the hydrological connectivity across the peatland watershed complex during early spring – a critical period where water table is elevated from snowmelt – using extended hydrological records from MEF (e.g., snow and frost depths, water table elevations, streamflow). Results show that (i) streamflow has decreased over decades due to increased evapotranspiration rates (despite no detectable trends in precipitation), (ii) the timing of spring water table recharge and streamflow is decoupled from shifts in snowmelt, and (iii) frost depth is a key explanatory variable for the timing and magnitude of streamflow. These results suggest that frost plays an important role in connecting surface water storage in peatlands to stream outlets, and that the hydrological connectivity across the peatland watershed complex can mediate the sensitivity of hydrological responses to climate variations.

References:

Feng, Xue, M. Julian Deventer, Rachel Lonchar, GH Crystal Ng, Stephen D. Sebestyen, D. Tyler Roman, Timothy J. Griffis, Dylan B. Millet, and Randall K. Kolka. "Climate sensitivity of peatland methane emissions mediated by seasonal hydrologic dynamics." *Geophysical Research Letters* 47, no. 17 (2020): e2020GL088875.

Title: **Model-Data Fusion to Examine Multiscale Dynamical Controls on Snow Cover and Critical Zone Moisture Inputs**

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Project Lead Principal Investigator (PI): Alejandro N. Flores

BER Program: ESS

Project: University Project

Project Website:

Project Abstract: Although the rate, spatial distribution, and magnitude of water delivery to Earth's critical zone presents a first order control on all subsurface biogeochemical processes, it is incredibly difficult to measure in the world's mountainous regions. Because the presence, longevity, and extent of seasonal snowpacks are a complex function of surface hydrometeorological conditions, it stands to reason that the ability to understand and model subsurface biogeochemical processes is directly related to the quality with which those forcings, particularly precipitation, are known. Commonly used mountain precipitation data can broadly be divided into three types: 1) applied interpolation techniques used to map sparse gauge observations across terrain, 2) statistical downscaling approaches to map coarse resolution atmospheric reanalyses to watershed-scales, or 3) dynamical downscaling, where physically based coupled land-atmosphere models are forced by atmospheric reanalyses as boundary conditions. The last decade has demonstrated that dynamical downscaling techniques are powerful tools for estimating both mountain precipitation inputs, and the related problem of modeling mountain snow accumulation. Evaluating output is a long-standing challenge, and one that is exacerbated in mountain regions where observations are sparse. Gridded datasets derived from surface observations can disagree substantially in mountain watersheds because of choices related to geostatistical methodologies. Moreover, there is often mutual dependence on these products and observations such that they are not entirely independent. Here we evaluate 34 years of Weather Research and Forecasting (WRF) model, version 3.8.1 precipitation output throughout a 700 km^2 mountain watershed (how high) in Colorado, using a combination of precipitation gauge observations, streamflow records, and a limited number of snow-lidar surveys (2018-2019). We also compare precipitation fields to gridded products. Basin-mean precipitation is also compared against precipitation-from-streamflow Bayesian inference method. This work builds upon prior research by incorporating lidar-derived snow water equivalent

estimates into the precipitation estimating framework. The developed forcing data is now available on the Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data-sharing platform [Rudisill et al., 2022].

References

Rudisill W; Vincent A; Nash C; Flores A (2022): Dynamically Downscaled (WRF) 1km, Hourly Meteorological Conditions 1987-2020. East/Taylor Watersheds. Science Area 1: Standard Award: Model-Data Fusion to Examine Multiscale Dynamical Controls on Snow Cover and Critical Zone Moisture Inputs, ESS-DIVE repository. Dataset. doi:10.15485/1845448

Remarkable diversity of metagenome-assembled genomes from key ammonia- and nitrite-oxidizing organisms recovered from hydrologically-variable floodplain sediments

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BER Program: ESS
Project: University project DE-SC0019119

Project Abstract: Subsurface microbial communities mediate biogeochemical transformations that drive both local and ecosystem-level cycling of essential elements, including nitrogen (N). Two functional guilds of chemoautotrophic microorganisms are responsible for the first oxidative step of the N cycle, nitrification: ammonia-oxidizing archaea (AOA) and bacteria (AOB) catalyze the oxidation of ammonia to nitrite, while nitrite-oxidizing bacteria (NOB) oxidize nitrite to nitrate. Despite the critical role nitrification plays in N-cycling and removal in terrestrial ecosystems, our understanding of the diversity, ecophysiology, and activity of nitrifying organisms in deeper soils/sediments is quite limited. To address this knowledge gap, our recent work examined the phylogenetic diversity and metabolic potential of subsurface ammonia-oxidizing Thaumarchaeota lineages in hydrologically-variable floodplain sediments in the Wind River Basin near Riverton, WY. Metagenomes obtained from 11 discrete depths along a ~2-m sediment profile at site KB1 yielded diverse Thaumarchaeota MAGs with distinct functional potential. Particularly notable was the shift in phylogenetic identity with depth, which appeared to be linked to soil moisture as well as C:N content. The predominantly 'terrestrial' *Nitrososphaerales* were dominant in the top, well-drained (dry) layers with relatively higher total C (and lower C:N), while the typically 'marine' *Nitrosopumilales* dominated the deeper, moister layers, including the capillary fringe where total C and N were lowest. All AOA MAG clusters shared the genomic potential for ammonia oxidation (e.g., AMO, NirK) and CO_2 fixation (e.g., 4-hydroxybutyryl-CoA dehydratase); however, surface soils were dominated by relatively more 'generalist' AOA capable of utilizing various organic compounds (e.g, urea, cyanate and nitriles), whereas 'oligotrophic' AOA lineages became prominent in deeper, moister layers.

We have also examined temporal changes in nitrifying communities within the soil/sediment column at a nearby Riverton site (Pit2), capturing a full seasonal floodplain hydrologic cycle of water table rise, flooding, and summer drought. Genome-resolved metagenomic analysis of these samples yielded 100 MAGs belonging to AOA (Thaumarchaeota) and 22 attributed to major NOB clades (*Nitrospinaceae*, *Nitrospirales*). Although some overlap was observed in AOA MAGs recovered from Riverton sites KB1 and Pit2, a surprisingly large number of AOA MAGs were found exclusively within Pit2 metagenomes; intriguingly, many of these were closely related to marine/estuarine *Nitrosopumilus* and *Nitrosarchaeum* species, as well as MAGs from estuarine sediments, suggesting adaptations to saline conditions may be shared among these AOA. Overall, this study is yielding unprecedented genomic and ecophysiological insights into subsurface nitrifying communities, over both time and space, in floodplain sediments directly influenced by hydrological fluctuations.

Remote Sensing of Plant Functional Traits for Modeling Arctic Tundra Carbon Dynamics

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BER Program: ESS
Project: University-Led Research
Project Website: N/A

Project Abstract:

Rapid warming in the Arctic is driving changes in the structure and composition of tundra vegetation communities. These changes are expected to alter key biogeochemical and physical processes that feedback to climate. However, the magnitude of this feedback is highly uncertain due to limited understanding of the spatial distribution of plant functional traits and the over-simplification of traits in current Earth system models. To facilitate improved representation of aboveground and belowground traits in models, we aim to characterize directly observable plant functional traits from remotely sensed data, and predict non-observable (e.g., belowground) traits by leveraging trait-environment relationships and trait covariation. Additionally, we will integrate trait information into the Terrestrial Ecosystem Model (TEM) to quantify and predict regional C balance in the Alaskan tundra.

In July and August 2021, we established four sites representing dominant plant community types in northern Alaska. Two sites were located south of the Brooks Range in the boreal-tundra ecotone, and the other two sites were in the Arctic Coastal Plain. In each site, we measured species percent cover, canopy height, and edaphic parameters, and collected leaf samples and root cores to characterize traits at the species, functional type, and community levels. Each site was also imaged with a drone to collect hyperspectral and LiDAR data. A minimum of six additional study sites will be sampled and imaged over the next two years. Using these data, we will test a range of hypotheses about the processes that control plant trait distributions in northern Alaska. We will also integrate ground-based measurements with information derived from multi-scale remote sensing platforms from drone, hypertemporal, LiDAR, and hyperspectral imagery to produce maps of leaf, size and root traits, greatly expanding the trait information available for modelers. Finally, we will use Bayesian data-model fusion methods to improve the parameterization and formulation of TEM, which is widely used in Arctic carbon studies, and perform simulation experiments to evaluate how differences in plant functional traits affect C dynamics.

Title: **Particulate Organic Matter (POM) Transport and Transformation at the terrestrial-aquatic interface**

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Project Lead Principal Investigator (PI): Matthew Ginder-Vogel

BER Program: ESS

Project: University

Project Website: N/A

Project Abstract: Over the past three years our ESS-SBR funded research has been examining particulate organic matter (POM) dynamics in near-surface sediments of the Columbia River through coupled field and lab experiments. Novel, riverbed "POM traps", designed cooperatively with the PNNL field team, were deployed in the near surface riverbed within the 300 Area. The deployment of these traps was timed to capture POM infiltration into riverbed sediments during low and high flow conditions. After deployment, materials from depth sections of each of three traps were wet sieved to obtain the fine-grained fraction (<250 μm) which was then analyzed in triplicate for POC/PON content. The trap deployments have revealed substantial POM accumulation in the upper 20 cm of sediment. Greater accumulation occurred during elevated river flow/elevation in June/July compared to February/March. Reactive transport simulations in which fluid flow and solute/colloidal POM transport were modeled using measured hourly hydrologic gradients between river and ground water provide an explanation for these results, where elevated rates of suspended POM-containing fluid flow into the riverbed lead to major POM accumulation through filtration and sorption processes. The boundary condition for suspended POM at the riverbed surface, as well as the POM filtration and sorption parameters, were constrained by a combination of in situ measurements, POM transport experiments and modest parameter fitting to produce estimates of POM accumulation that approximated observed levels of accumulation in the POM traps. Enhanced POM accumulation during periods of high fluid influx to the riverbed releases soluble labile DOC whose coupled transport and metabolism lead to periods of pore fluid dissolved oxygen (DO) depletion. These results provide a compelling illustration of how in situ (i.e. field-scale) experimentation can be coupled with modeling (i.e. the ModEx paradigm) to reveal system feedbacks and dynamics.

Where Do Inflows Occur Along Western Rivers? Using Water Quality Profiles and Geophysics to Identify Inputs to Rivers

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Project Lead Principal Investigator (PI): Michael Gooseff

BER Program: ESS

Project: University Project; *Resolving Aquifer Controls on Larger River-Groundwater Exchanges of Mass and Energy*

Project Website:

Project Abstract:

Groundwater inflows to rivers are controlled by both the hydraulic head gradients between the channel and surrounding aquifer and the spatial distribution of hydraulic conductivity in the subsurface. In this project we seek to determine how the spatial distribution of geologic units influences the locations of groundwater inflows to western rivers, namely the Columbia River in Eastern Washington, the Colorado River in Colorado, the Green River in Utah, and the Gunnison River in Colorado. To date we have collected high-frequency water quality data in the water column and along the beds of these rivers to identify locations of anomalies indicating the inflows of water that is different in character than channel water. In the case of the Columbia River, we have also collected transient electromagnetic (TEM) geophysical data along the river to map changes in subsurface resistivity (using the boat-pulled FloaTEM system), indicative of changes in geologic units. Preliminary assessment of summer 2021 data collection from the Columbia River shows promise that a set of inflows identified by the water quality survey align with shifts in resistivity identified by the FloaTEM data. Others that do not align are likely associated with surface controls (e.g., irrigation return flows). In the case of the Colorado, Green, and Gunnison Rivers, very few anomalies were identified, perhaps because of the low flow conditions in 2021. Samples collected for water stable isotope analysis from these rivers demonstrate a strong evaporation signal. Dissolved radon analyses suggest little 'old water' contributions to these rivers.

Title: Effects of Microbial Growth and Death and Sediment Movement on Hyporheic Zone Biogeochemistry

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BER Program: Environmental System Science

Project: Effects of Surface Water Fluctuations and Sediment Movement on Hyporheic Zone Biogeochemistry and Microbial Communities (University project)

Project Abstract: The hyporheic zone beneath and adjacent to river channels is often more reactive than overlying surface water or deeper groundwater, and thus is an important area for chemical transformation within watersheds. This exploratory project developed a predictive mechanistic modeling approach to quantify the effects of microbial growth and death processes as well as bed sediment migration on hyporheic zone microbial populations and biogeochemical cycling. We focus on 1) baseflow conditions which are most common and sediment migration is well understood, and 2) riverbed dunes which are widespread in larger streams and rivers and often dominate hyporheic effects on water quality. We linked a series of existing models that simulate surface water hydrodynamics (OpenFOAM), groundwater flow (MODFLOW), and groundwater transport/reaction and microbial growth/death (SEAM3D). We developed and tested a moving frame of reference (MFOR) approach to simulate dune migration effects on biogeochemical transformations through modification of SEAM3D. We then conducted sensitivity analyses of controlling factors such as hydraulic, sediment, biogeochemical, and microbial model parameters and boundary conditions. For our results without dune migration, biomass reached a steady state in every simulation within ~ 2 days model time, and increased with hyporheic flow cell area as controlled by hydraulic boundary conditions. Not accounting for microbial growth and death tended to underestimate steady-state microbial biomass and DO/DOC consumption and overestimate DO/DOC concentrations. Increasing steady-state DOC availability caused the microbial population to grow more than did increasing steady-state DO availability. Decreasing DO availability, on the other hand, caused more microbial death than decreasing DOC availability. We also found that there are minimum DO and DOC steady-state concentrations required for microbial growth. Varying both hydraulic and biogeochemical steady-state boundary conditions affected spatial distribution of biomass, DO and DOC. Our results with dune migration are more preliminary, but indicate that dune migration reduced microbial populations dramatically relative to static dunes. This effect increased with dune celerity, while residence times and contaminant removal simultaneously declined. Overall, our results indicate that accounting for dynamics of both microbial growth/death and sediment movement can be important for correctly predicting the magnitude of hyporheic biogeochemical transformations, with important implications for material processing in watersheds.

Title: Testing Mechanisms of How Mycorrhizal Associations Affect Forest Soil Carbon and Nitrogen Cycling

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Project Lead Principal Investigator (PI): Caitlin Hicks Pries

BER Program: ESS

Project: University-led research

Project Website: NA

Project Abstract: Mycorrhizal fungi provide plants with nutrients in return for photosynthate, linking above and belowground processes. Forests dominated by arbuscular (AM) versus ectomycorrhizal (EcM) fungi have well-documented differences in their distributions of soil carbon (C) and nitrogen (N). However, the mechanisms driving these patterns are uncertain. Potential mechanisms include differences in leaf litter quality and nutrient acquisition strategies. Some EcM fungi acquire N from organic matter by producing their own extracellular enzymes. This strategy may lead to the "Gadgil Effect" whereby competition between EcM fungi and saprotrophs limits decomposition. In contrast, AM fungi are limited to scavenging nitrogen from the soil solution, which may lead to increased root exudation in AM forests. We are testing how differences in litter quality or nutrient acquisition strategies affect the distribution of C and N within mineral soil using isotopic labeling experiments and updates to the CORPSE model. We are currently incubating six different types of dual ^{13}C and ^{15}N-labeled litter in soil mesocosms at forests in NH, IL, and GA where each have six plots differing in the abundance and dominant family of EcM-associated trees. We also performed a greenhouse experiment wherein eight species of seedlings (four AM and four EcM) were grown in a ^{13}C-labeled atmosphere under three levels of N fertilization to trace how mycorrhizal type and N availability affect the fate of root and hyphal exudates in soils and the priming of native soil decomposition. Thus far, we have found that the amount of new photosynthate in the soil increased with EcM plant biomass but not AM, and that soil microbial biomass decreased with increasing N availability in EcM but not AM soils. We have updated the CORPSE model to include different mycorrhizal nutrient acquisition strategies so that EcM fungi can mine soil organic matter for N, but AM fungi cannot. We used the model to explore the conditions under which EcM fungi can induce saprotrophic N limitation (i.e., the Gadgil effect). We found that the Gadgil effect is strongest in

ecosystems with high seasonality in temperature and litterfall, such as temperate deciduous and boreal evergreen forests. However, the Gadgil effect does not strongly affect soil carbon storage. This ongoing research is bringing new insights into the mechanisms driving mycorrhizal differences in soil organic matter cycling.

Title: **Modelling Microbes to Predict Post-fire Carbon Cycling in the Boreal Forest across Burn Severities**

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Project Lead Principal Investigator (PI): Dr. Thea Whitman

BER Program: ESS

Project: University

Project Abstract: Boreal forests hold large amounts of carbon (C) above- and belowground, making them a major reservoir of C globally. In North American boreal ecosystems, wildfire is the primary stand-replacing disturbance, and fires are projected to increase in frequency and severity, which could affect microbial community composition and soil C cycling. However, data quantifying the effect of wildfire on soil community and C storage are sparse, and our understanding of the mechanisms driving these effects remains limited. Recent advances in biogeochemical model representations of soil C cycling, such as the Carbon, Organisms, Rhizosphere and Protection in the Soil Environment (CORPSE) model, have an emphasis on explicitly representing the system in an increasingly mechanistically accurate way. In our project, we aim to determine whether linking belowground microbial community composition, size, and activity to aboveground properties of burn severity and plant community composition allows us to better model post-fire soil carbon dioxide (CO_2) fluxes using the CORPSE model. In burn simulations on soil cores, we found that higher temperature burns led to larger shifts in bacterial community composition, which were accompanied by shifts toward taxa with higher predicted weighted mean 16S rRNA gene copy numbers and proportionally smaller fast-cycling C pools. Using laboratory incubations, we empirically identified fire surviving and fast growing bacterial taxa, as well as taxa with an affinity for the post-fire soil environment and then analyzed the importance of these fire adaptive strategies in field data one and fire years after natural wildfires of varying severities. The relative importance of these three strategies varied with time, burn severity, and soil depth. In the next step of this project, we will use burn simulations in intact soil cores, post-burn incubations, and corresponding measurements of CO_2 emissions, C use efficiency, and microbial biomass paired with microbial community composition to build and test models of post-fire soil CO_2 fluxes. We will compare the abilities of a low-complexity model based on fast and slow C pools, a mid-complexity model that considers C protection mechanisms and microbial biomass, and a high-complexity model, which incorporates microbial fire-adapted strategies, to predict post-fire soil CO_2 fluxes.

Title: **What Drives Variability in Carbon-Water Dynamics? The Value of Soil Moisture for Predicting Plant Water Potential and Ecosystem Fluxes**

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Project Lead Principal Investigator (PI): Steven Kannenberg

BER Program: ESS

Project: University project

Project Website: NA

Project Abstract:

Carbon and water fluxes in arid and semi-arid ecosystems are notoriously difficult to predict due to their high spatial and temporal variability, and progress towards this aim is limited by the accuracy and resolution of existing data. In particular, measurements of shallow and deep soil moisture pools have the potential to greatly enhance our ability to predict ecosystem fluxes. Additionally, data on plant water potential (WP) could improve predictions of ecosystem fluxes since plant hydraulic status acts as the intermediary between soil and atmosphere. However, the sensitivity of ecosystem fluxes to atmospheric drivers, soil WP, and plant WP remains unresolved. We addressed this challenge using co-located continuous measurements of soil WP profiles, tree WP (via stem psychrometers), and ecosystem fluxes (via eddy covariance) at a site in southeastern Utah, along with a broader network of 21 arid flux tower sites in the western US where soil moisture has been monitored at multiple depths.

We found that ecosystem fluxes of carbon and water were highly sensitive to variability in soil WP, especially in shallow (<20 cm) layers. The sensitivity of fluxes to shallow soil WP greatly exceeded flux sensitivity to vapor pressure deficit, air temperature, and solar radiation, even in ecosystems dominated by deep-rooted woody vegetation. Tree WP was also most sensitive to shallow soil WP, and was tightly linked to ecosystem-scale carbon and water fluxes. However, using a model comparison exercise, we found that the inclusion of tree WP data did not improve predictions of modeled fluxes any more than the addition of just one layer of soil WP. Instead, we found that the inclusion of any additional depths of soil WP improved model fit. Our results indicate that prediction of ecosystem fluxes and plant WP can be greatly enhanced via denser networks of soil moisture observations and novel remotely-sensed soil moisture products (e.g., SMAP), especially in arid and semi-arid ecosystems with highly variable hydrological cycles.

The Impact of a Changing Permafrost Tundra Ecosystem on Dissolved Organic Carbon Age and Concentration in Surface and Groundwater in a Long-Term Experiment

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BER Program: TES
Project: University, Schuur
Project Website: http://www2.nau.edu/schuurlab-p/CiPEHR.html

Project Abstract: New estimates place 1440-1600 billion tons of soil carbon in the northern circumpolar permafrost zone, more than twice as much carbon than in the atmosphere. Understanding the magnitude, rate, and form of greenhouse gas release to the atmosphere is crucial for predicting the strength and timing of this carbon cycle feedback to a warming climate. Here we report results from an ecosystem warming manipulation where we increased air and soil temperature and degraded the surface permafrost. We used snow fences coupled with spring snow removal to increase deep soil temperatures and thaw depth (soil warming) and open top chambers to increase growing season air temperatures (air warming). The soil warming treatment has successfully warmed soils by 2-3ºC in winter, increased growing-season depth of ground thaw by up to 200%, and degraded an increasing amount of surface permafrost each year of the project. The primary drivers of the tundra ecosystem carbon balance across the Arctic landscape, air temperature, deep soil temperature, permafrost extent, and soil moisture were manipulated as a result of experimental warming. The water table was also altered, as the ground surface subsided below the top of the water table in some plots and along with increased thaw resulted in for deeper, older layers of the soil profile to become saturated with surface water perched on the permafrost. Here we report measurements of long-term dissolved organic carbon (DOC) leaching as a metric of changes in ecosystem carbon storage. Warming increased carbon exchange with soil water, increasing DOC concentrations in warmed plots by an average of 130% to 93mg/L in warmed plots as compared to 40mg/L in control plots. There was also an observed depletion in DOC-$\Delta^{14}C$ with warming, with $\Delta^{14}C$ values as low as -320‰. This value corresponds to a mean radiocarbon age of ~3,000 years, but actually is likely to represent a mix of modern and much older, permafrost C. The oldest DOC mixtures were located in deeply thawed, warmed tundra whereas younger carbon from freshly decayed soils and plants was present in less deeply thawed portions of the tundra. Permafrost carbon with values as low as -200‰ was also detected in surface water downstream from the experimental site, particularly after large rain events. These findings indicate that permafrost carbon is vulnerable to leaching and is likely to enter aquatic ecosystems following mobilization from terrestrial permafrost soil. This process is irreversible and likely to further exacerbate climate change.

Title: **Carbon transformation and transport in a high elevation mountain catchment**

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Project Lead Principal Investigator (PI): Li Li

BER Program: ESS

Project: Advancing a Watershed Hydro-biogeochemical Theory: Linkage between Water Travel Time and Reactive Rates Under Changing Climate [University project, lead PI, Li Li, Penn State)

Project Abstract:

Mountain areas are warming up faster than lowland places, imposing tremendous implications to soil biogeochemical reactions, water availability and chemistry, and climate-carbon feedback. Dissolved organic and inorganic carbon (DOC and DIC), as well as soil CO_2, are produced in soils and exported from soils to streams, where CO_2 evasion emits a sizable portion of CO_2 comparable to the emission of soil CO_2 to the atmosphere. The magnitude and drivers of dissolved carbon in the fast-warming mountain areas however are poorly understood[1, 2]. Here we ask the question: how and to what extent does warming affect flow paths, carbon biogeochemical reactions, and its export in mountain streams? To address the equation we used watershed-scale reactive transport modeling and stream flow and chemistry data collected every other day for multiple years in a high elevation mountain watershed, Coal Creek, in Colorado. Analysis of stream data reveals occurrence of high DOC concentrations during high flow times and high DIC concentrations during low flow times. The watershed-scale reactive transport model was used to simulate flow paths, soil respiration, and carbon decomposition in the subsurface, and to understand and quantify rates and drivers of carbon transformation and transport. Modeling results suggest significant DOC and soil organic matter mineralization in longer and deeper groundwater flow paths, resulting in reduced DOC and increased DIC concentrations in deep ground water compared to shallow soil water. Results indicate carbon transformation in the deep subsurface can contribute substantially to the dissolved carbon in deep ground water and in streams. This suggests that even though oxygen and organic matter availability are lower in deep subsurface, carbon decomposition may be still significant due to its longer flow paths and longer water residence time for processing carbon.

Publications:

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2. Zhi, W.; Li, L.; Dong, W.; Brown, W.; Kaye, J.; Steefel, C.; Williams, K. H., Distinct Source Water Chemistry Shapes Contrasting Concentration-Discharge Patterns. Water Resour. Res. **2019,** 55, (5), 4233-4251.

Rewriting the Redox Paradigm: Dynamic hydrology shapes nutrient and element transformations in a Great Lakes coastal estuary

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BER Program: ESS
Project: University-led "Rewriting the Redox Paradigm: Dynamic hydrology shapes nutrient and element transformations in a Great Lakes coastal estuary" (DE-SC0022191)
Project Website: N/A

The propensity for redox processes to occur is sometimes predicted by measured or assumed redox potential (E_h), but process measurements often deviate from predictions based on the thermodynamic "redox tower" paradigm. We hypothesize that poorly measured, granular scale soil heterogeneity causes apparent departures from thermodynamic exclusion principles at bulk scales, with consequences for biogeochemical cycling which are not currently resolved in ecosystem, regional, or global scale models. We will combine empirically measured traditional biogeochemical indicators with newly developed electrochemical approaches to determine how fluctuating hydrology shapes redox regimes and processes. Specifically, our objectives are to (1) relate dynamic hydrology in a freshwater terrestrial aquatic interface wetland (Old Woman Creek, OH) to redox regimes; (2) determine how redox heterogeneity drives elemental cycling at multiple scales, and; (3) assess the sensitivity of process-based models to the inclusion of fine-scale variability in redox conditions. We will use zero resistance ammetry (ZRA) to exploit redox disequilibria among discrete zones to detect the distributions, extents, and kinetics of biogeochemical processes. ZRA can measure electrical current that arises from microbially-induced redox disequilibrium. In winter 2021-2022, we worked to refine a paired ZRA and Eh multi-sensor system that will detect electrochemical signals across the sediment-water interface at nested scales (sub-millimeter to decimeter) at a shallow location (< 10 cm surface water) in the Old Woman Creek wetland. In summer 2022, we will deploy these sensors and collect concurrent data on dissolved oxygen dynamics, surface and pore water nutrient concentrations, greenhouse gas fluxes (chamber measurements), and soil geochemistry. We will then use those data to demonstrate the feasibility of integrating microsite electrochemical and redox variability to the ecosys ecosystem scale model for improved representation of soil redox processes in spatially variable and temporally fluctuating systems.

Title: **Fungal Response to Multiple Global Change Stressors: Evidence from Long-Term Manipulations and Environmental Gradients**

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Project Lead Principal Investigator (PI): Stephanie N. Kivlin
BER Program: ESS
Project: University Project

Project Abstract:
Global change is affecting terrestrial ecosystems in multiple ways. In mountain ecosystems, direct effects (e.g., raised soil temperatures) and indirect effects (e.g., early snowmelt, decrease in snowpack) of warming are co-occurring. Our ability to forecast belowground responses to these complex global change drivers has been hindered by a lack of long-term studies. Yet, these belowground studies are vital as soil fungi are key decomposers in terrestrial ecosystems, potentially flipping soils from carbon sinks to carbon sources. Here we examined soil fungal responses (composition and abundance) to a 29-year-long warming experiment and a 4-year-long early snowmelt manipulation at the Rocky Mountain Biological Laboratory in Gothic, Colorado in 2019-2021. These data were paired with those collected the same year from nearby environmental gradients in temperature (e.g., elevation) and snowmelt date (e.g., at different slopes and aspects). These approaches are complementary. Environmental gradients capture long-term ecological and evolutionary variation but can be confounded by many covarying abiotic and biotic factors. Long-term experiments allow us to understand the role of a specific global change driver but may not occur over long enough time periods to capture both ecological and evolutionary responses.

Soil fungal communities varied substantially in response to abiotic environmental gradients. Up to 8% of the variation in fungal composition was explained by elevation (a long-term proxy for temperature) and 15% of variation in fungal composition was explained by aspect (a long-term proxy for snowmelt date). Snowmelt date in the collection year explained an additional 10% of variation in fungal composition. Experimental treatments affected fungal communities less. Experimental early snowmelt explained 6% of the variation in fungal communities whereas warming only explained 4% of the variation in fungal communities. Fungal abundance followed similar trends with hyphal lengths varying the most by elevation and aspect, and the least in experimental manipulations. Overall, our results suggest that fungi are more sensitive to historical and contemporary snowmelt date (which varies by 56 days since 1975) than the direct effects of warming per se. Because fungal response to snowmelt is strong, and snowpack and melt dates are highly variable, future ecosystem models may be improved by including fungal functions across the transition in snow cover. Future research in our group is focused on comparing plant, fungal, and biogeochemical phenology in response to snowmelt date.

Title: Toward a predictive understanding of environmental perturbations in regulating greenhouse gas release in northern peatlands

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Project Lead Principle Investigator (PI): Joel E. Kostka

BER Program: ESS

Project: University project

Project Website: Affiliated with SPRUCE; https://mnspruce.ornl.gov/

Project Abstract:

Our project goal is to develop a mechanistic understanding of how environmental disturbance (warming, eCO_2, drought, plant community shifts) regulates microbial communities, soil organic matter(SOM) decomposition and greenhouse gas emission rates and ratios from peatlands. Our team has compiled a 7-year time series of the concentrations and isotopic composition ($\delta^{13}C$ and $\delta^{14}C$) of major carbon species (solid peat, porewater CO_2 and CH_4, dissolved organic carbon), metabolites, enzyme activities, and microbiomes in the experimentally warmed SPRUCE peatland which includes experimental manipulation of CO_2(eCO_2).

Warming induced changes in the plant community and resulting organic matter inputs were correlated with increasing CO_2 and CH_4 production. Lipids significantly increased with both temperature and eCO_2, and lipids/sugars were also a significant predictor of CH_4/CO_2 ratio, suggesting that a shift towards increasing abundance of shrubs will further promote methanogenic conditions. Mass-balance modeling of isotopic data revealed increases in solid peat-supported respiration in heated plots over time and relative to ambient enclosures. The following contrasts were observed in the ambient vs. eCO_2 enclosures: $\delta^{13}CH_4$ is significantly more depleted, CH_4/CO_2 concentrations are marginally greater, and $DI^{14}C$ was depleted relative to the controls in the eCO_2 plots. Peat microbial communities appeared stable over 7 years; however, only limited replication was possible due to the destructive nature of soil coring. Thus, we developed methods for higher frequency sampling of planktonic microbial communities in porewater and observed a significant decline in diversity along with a substantial shift in community composition with warming. Finally, we investigated the response/recovery of microbial community enzyme activity to a generational drought in summer of 2021; while no response was observed in hydrolase activity, phenol oxidase activities were elevated in warmer and drier soils during the drought.

Our results suggest that as climate forcings worsen, peatland systems will become increasingly methanogenic, resulting in a positive feedback loop that exacerbates climate warming. We are just beginning to see statistically significant changes in microbial community dynamics and a stimulation in the respiration of ancient catotelm peat C, deposited under prior climate(cooler) conditions. Shifts in microbial diversity and community composition point to a loss of stability with warming, with potentially dramatic implications for ecosystem functioning. The apparent destabilization of the large peat C reservoir has substantial implications for

peatland-climate feedbacks. After a ~5 year lag, we also observe a significant influence of eCO_2 on the reactants and products of organic matter mineralization suggesting a synergistic effect between temperature and eCO_2.

References:
[1] Wilson, R. M., Griffiths, N. A., Visser, A., McFarlane, K. J., Sebestyen, S.D., Oleheiser, K. C., Bosman, S., Hopple, A.M., Tfaily, M.M., Kolka, R.K., Hanson, P.J., Kostka, J.E., Bridgham, S.D., Keller, J.K., and J.P. Chanton. (2021). Radiocarbon analyses quantify peat carbon losses with increasing temperature in a whole ecosystem warming experiment. Journal of Geophysical Research: Biogeosciences,126, e2021JG006511. https://doi.org/10.1029/2021JG006511

Development of a molecularly informed biogeochemical framework for reactive transport modeling of subsurface carbon inventories, transformations and fluxes

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Project Lead Principal Investigator (PI): Kate Maher

BER Program: ESS

Project: University Project

Project Abstract:

To understand how soils moderate heterotrophic and autotrophic respiration of CO_2, our project is using field and laboratory measurements of soil respiration, soil pCO_2 and soil organic carbon (SOC) content across the montane to sub-alpine ecosystems of the Rocky Mountain Biological Laboratory surrounding Gothic, CO watershed. Given the importance of exchanges across scales for improving modeling abilities, our project considers soil functional complexity in three conceptual dimensions: temporal variability, molecular diversity and spatial heterogeneity. Along the temporal axis of variability, we find that model structures that account for dormancy in response to pulsed wetting events, as well as plant phenology (*e.g.*, senescence) are critical for capturing the response of soil respiration to changes in the timing and magnitude of both snowmelt and the summer monsoonal precipitation. In terms of molecular diversity, we extended the SOC functional group abundance (SOC-fga) method that combines Fourier transform infrared spectroscopy (FT-IR) and bulk carbon X-ray absorption spectroscopy (XAS) to evaluate the density fractions within multiple meadow depth profiles. We find site-to-site variations in light and occluded fractions that contrast with the consistency in the heavy fraction between sites (polysaccharide and amide), indicating that regardless of carbon input, the residual products of SOC turnover have very similar structures, possibly due to sorption on mineral surfaces. In terms of spatial heterogeneity, we have combined airborne remote sensing with ground-truth SOC inventories to map the spatial heterogeneity in soil carbon. We find that depositional zones, including floodplains and fens, have an outsized control on carbon accumulation, but are difficult to predict based on topographic constraints alone. In these environments, we also find evidence for active methane cycling that shifts the functional complexity, pointing to a need for better characterization to understand how their temporal response and molecular diversity compares to the hillslope sites. Collectively, our results indicate that the spatially averaged fluxes may not equate to fluxes calculated for the averaged compartments, requiring consideration of not only the soil functional complexity but the upscaling methods used to represent it.

Title: **Identifying Hot Spots and Hot Moments of Metabolic Activity in Salt Marsh Sediments Through BONCAT-FISH Microscale Mapping**

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Project Lead Principal Investigator (PI): Jeffrey Marlow

BER Program: ESS

Project: University project

Project Abstract: Complex microbial communities are essential constituents of soil and sediment ecosystems: they modulate nutrient and metabolite flux in ways that filter runoff, determine greenhouse gas emissions, and support higher trophic levels. However, our ability to derive net biogeochemical fluxes from knowledge of a community's constituents is limited by a lack of suitable methods connecting metabolic activity on a single-cell level to bulk processes. In salt marsh sediments, where redox zones are compressed due to substantial organic loading, this challenge is particularly pronounced: connections between dominant electron-donating (carbon) and electron-accepting (sulfur) metabolic cycles lack spatial and temporal specificity.

Our work to identify the "hot spots" and "hot moments" of metabolic activity in salt marsh sediment follows up on recent efforts conducting *in situ* substrate analog probing incubations in Little Sippewissett Salt Marsh in Falmouth, MA. Through the development of customized incubation chambers, we exposed intact sediment columns to the substrate analog L-homopropargylglycine (HPG), which is incorporated into growing biomass and subsequently visualized through click chemistry and fluorescence microscopy. The approach is known as bio-orthogonal non-canonical amino acid tagging (BONCAT); initial work revealed growing microbes in precise spatial arrangements with respect to specific mineral grains (Marlow et al., *Environmental Microbiology*, 2021).

The next steps are to gain additional temporal and phylogenetic resolution on which organisms are active under distinct conditions. Here, we share preliminary results of a two-phase BONCAT technique, as well as background spectral profiling to enable optimized fluorescence microscopy analysis. Using both HPG and a different substrate analog (L-azidohomoalanine, AHA), we have developed a novel method to visualize anabolically active organisms under two different environmental conditions, doubling BONCAT's temporal resolution and revealing which community members are growing during the day or night. In preparation for multiplexed fluorescence *in situ* hybridization (FISH), we have developed microscale maps of salt marsh sediment spectral profiles under UV/vis excitation. These spectral maps, developed with sub-micron spatial resolution, will indicate which spectral windows are most promising for FISH. We have also incorporated fluorescence lifetime data into this map, offering an additional "dimension" of differentiation to both characterize the substrate and guide fluorescence analysis.

These efforts have set the stage for a late summer field deployment to further resolve the "hot spots" and "hot moments" of microbial activity, offering a promising opportunity to link single-cell activity with broader environmental biogeochemical processes.

Title: **Unraveling the Mechanisms of Below- and Aboveground Liana-Tree Competition in Tropical Forests**

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BER Program: ESS

Project: University Project

Project Website: n/a

Project Abstract: Trees and lianas dominate the canopy of tropical forests and comprise the majority of tropical aboveground carbon storage. These growth forms respond differently to variation in climate and resource availability, and their responses to future climate change are poorly understood. The objectives of this project are to carry out an observational campaign to advance our understanding of liana traits and strategies, develop a liana-enabled forest dynamics model that leverages our observations, and to engage with the Earth System Modeling (ESM) community to plan for the eventual inclusion of lianas into ESMs. Here, we report on six activities from the past year. (1) We measured and conducted meta-analysis of liana traits. On average, we found marked differences between lianas and trees in terms of their hydraulic traits and xylem anatomical traits. We also identified significant variation in hydraulic traits across liana species. (2) We incorporated these results into a model, and subjected the model to different tropical hydroclimate scenarios. Due to differences in hydraulic conductivity, the model indicated that lianas are much more susceptible than trees to reaching a hydraulic threshold for viability by 2100. (3) We measured tree growth and liana colonization status of over 1,700 trees at a study site in Guanacaste, Costa Rica. We found that the number of colonized trees is increasing and that heavily infested trees have lower relative growth rates that other trees. Liana colonization also impacted the relationship between tree growth and rainfall. (4) We incorporated lianas into the TROLL forest dynamics model and developed new schemes for leaf production and turnover. We have carried out a sensitivity analysis and variance decomposition with respect to model parameterization. We found that the sensitivity to the leaf production scheme is greater than the sensitivity to leaf turnover. (5) We implemented liana-enabled forest dynamics in TROLL. These dynamics include the ability of lianas to colonize an arbitrary number of trees in its neighborhood and the ability of trees to shed lianas. (6) We are measuring litterfall and fine root production in the plots. We installed 30 cm deep root ingrowth cores in 18 plots in December 2020 and May 2021 We are further partitioning fine root production into lianas versus trees using molecular analyses. We have begun preliminary tests to optimize the primers and PCR conditions for the molecular analyses.

Advective Heat Transport in Permafrost Landscapes: Biogeochemical Consequences

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BER Program: TES
Project: University project

When ice-rich permafrost thaws, the ground subsides, creating thermokarst features such as thaw bogs. These bogs are topographic low points in the landscape, and thus they receive and collect subsurface runoff from surrounding permafrost peat plateaus. The hydrologic connection between permafrost plateaus and thaw bogs has the ability to increase bog methane emissions by transporting thermal energy and nutrients from the plateau into the bog. On the time scale of interest for climate predictions (decades to centuries), radiative forcing associated with thermokarst bog formation is largely dictated by the amount of emitted methane.

Data previously collected by the research team from a thaw bog in Interior Alaska demonstrated that rainfall early in the growing season notably increased CO_2 uptake and CH_4. Water from the surrounding permafrost-peat-plateau flowed through the peat soils and penetrated into the bog, rapidly warming bog soils down to deep depths (~80 cm). The warm, deep bog soils early in the growing season supported microbial and plant processes that enhanced CO_2 uptake and CH_4 emissions. These results highlight how the plateau-bog hydrologic connection can influence methane. However, the hydrologic connection between bogs and the surrounding permafrost plateaus, and the ability of this connection to impact biogeochemical processes in the bog, is not traditionally recognized in field studies nor included in models.

Our project is advancing understanding of the bog-watershed connection, clarifying the conditions under which it results in the transport of thermal energy into bog and impacts land-atmosphere exchange of carbon. We are conducting fieldwork at a well-instrumented, thawing bog complex in Interior Alaska and performing Earth System modeling. Field data thus far indicate that bogs that receive proportionately more water from the surrounding watershed emit more methane. Through coupled modeling of lateral water and heat transport with Energy Exascale Earth System Model (E3SM) land model (ELMv1-ECA), we have confirmed the important role of advective heat transport in affecting bog soil temperatures and CH_4 emissions. Specifically, results show that incorporating lateral advective heat transport improved simulated soil-temperature and moisture profiles, active layer thickness (ALT), and bog inundation dynamics. Further, simulations that consider advective heat transport demonstrate deeper ALTs at bog edges than those without advective heat, suggesting advective heat transport facilitates faster thermokarst expansion.

Northern latitudes are expected to get warmer and wetter, and initiation and expansion of thermokarst thaw is expected to increase. In this context, the influence of the bog-watershed connection is likely to increase.

Title: High-Frequency Greenhouse Gas Emissions from a Coastal Wetland

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Project Lead Principal Investigator (PI): Genevieve Noyce

BER Program: ESS

Project: University project

Project Abstract:

The dynamic nature of the coastal terrestrial-aquatic interface (TAI) means that the processes the regulate decomposition and greenhouse gas (GHG) emissions are of particular significance to incorporate into Earth systems models. Despite this, we have a limited mechanistic understanding of how climate stressors interact with biological components to regulate the electron acceptors and donors that determine decomposition pathways within TAIs. Accurately modeling these processes is critical for incorporating the coastal TAI in Earth systems models, but doing so requires a better understanding of the processes that couple climate stressors, decomposition pathways, and net primary productivity in order to characterize feedbacks between biological, physical, and biogeochemical processes.

In 2021, we installed a network of 12 linked chambers in a mixed vegetation community in Smithsonian's Global Change Research Wetland, on an estuary of the Chesapeake Bay. These chambers automatically measure methane (CH_4) and CO_2 fluxes, with each chamber closing every 72 minutes during the growing season and every 132 minutes during the winter. Since system was started in April 2022, we have measured GHG fluxes from plant emergence to senescence, over soil temperatures ranging from 0 – 25 °C, and over water depth ranging from 80 cm above the surface to 20 cm below the surface. This wide range of data allows us to identify, and thus model, environmental conditions that lead to "hot moments", with the ultimate goal of using these data to improve modeling of decomposition and CH_4 cycling in PFLOTRAN. Methane fluxes exhibited strong seasonal effects, as expected, but also unexpected diurnal trends. Preliminary results suggest that CH_4 fluxes from this site are higher and more variable overnight than during the day, potentially due to shifting patterns of CH_4 oxidation or transport. Vegetation composition and flooding conditions also affected the magnitude and dynamics of CH_4 emissions. In February 2022, we added 1.5 m of soil heating to the automated chamber system; the chambers now span a range from ambient soil temperature to 6 °C above ambient. During the first three weeks of warming, GHG fluxes from the heated chambers were noticeably higher than ambient fluxes; we will continue assessing changes in GHG dynamics over the growing season, including how warming interacts with flooding and vegetation dynamics.

Title: **Temperature and Elevated CO_2 Effects on Coastal Wetland Resilience and Carbon Accumulation**

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BER Program: ESS

Project: University project

Project Website: https://serc.si.edu/gcrew/warming

Project Abstract:

Coastal wetlands are hotspots of carbon sequestration that regulate the biogeochemistry of coastal rivers, estuaries, and continental shelves, yet these ecosystems are highly vulnerable to global change. The Salt Marsh Accretion Response to Temperature eXperiment (SMARTX) was established at the Smithsonian's Global Change Research Wetland in 2016 to advance model representations of the complex interactions between plants, microbes, and hydrology in forecasts of coastal wetland responses to global climate change. We actively manipulate whole-ecosystem temperature through feedback-controlled heating from the plant canopy to 1.5 m soil depth as well as atmospheric CO_2 concentration.

Warming temperatures may increase wetland productivity and organic matter accumulation, but feedbacks between productivity and decomposition make it difficult to model how wetlands will respond to climate warming. A moderate amount of warming (1.7 °C above ambient) consistently maximized marsh elevation gain and below-ground carbon accumulation since the beginning of the experiment, consistent with our previously-observed non-linear effects on belowground net primary productivity. At higher temperatures, marsh elevation loss increased and was associated with increased carbon mineralization and microtopographic heterogeneity, a potential early warning signal of marsh drowning.

Elevation gain was highest in the wetter site, offering empirical support to our previous numerical modeling suggesting that the positive impacts of temperature on marsh carbon accumulation are maximized at high rates of sea-level rise, but also highlighting that warming-

induced gains in one part of the system may be offset by losses elsewhere. Elevation was also consistently maximized in early spring and minimized in the fall, which we attribute to seasonal changes in organic matter accumulation. The observed summer elevation loss indicates that, under warming conditions, the balance between decomposition and production is largely negative, with high rates of decomposition (inferred from methane emissions) reducing organic matter storage. This likely interacts with plant effects, where high root growth during the summer brings in oxygen and organic carbon, increasing rates of decomposition.

Elevated CO_2 also stimulated changes in plant morphology that led to a decline in carbon accumulation, especially when combined with warming, despite increased inputs of belowground primary productivity. This indicates that enhanced root production under future climate conditions may not increase marsh resilience, due to feedbacks resulting in high rates of aerobic decomposition. In addition, even though elevated CO_2 also reduced methane emissions, it did not substantially alter the radiative forcing potential of the marsh, due to the decrease in soil carbon sequestration.

Title: **Investigating Riverine Freshwater and Dissolved Organic Carbon Exports Across the Western Arctic Through Integration of Measurements and Modeling**

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Project Lead Principal Investigator (PI): Michael Rawlins

BER Program: ESS

Project: University project

Project Abstract:

This project aims to advance understanding of lateral land-ocean flows of freshwater and dissolved organic carbon (DOC) to coastal zones in Arctic regions. Manifestations of climate change in the Arctic are numerous and include hydrological cycle intensification and permafrost thaw, both expected as a result of atmospheric and surface warming. Field sampling, however, is too often of limited duration to confidently ascertain long-term trends in freshwater and nutrients flows to coastal waters. We use observations and numerical modeling to investigate influences on the fluxes and characterize their spatial and temporal dynamics, export magnitudes, and contemporary and future trends. We recently developed new algorithms for the mobilization and export of riverine DOC in a modeling framework that centers on application of a process-based permafrost hydrological model and digital flow direction network. Model validation leverages data from field measurements, synthesis studies, and modeling studies. The simulations effectively quantify DOC leaching in surface and subsurface runoff and broadly capture the seasonal cycle in DOC concentration and mass loading reported from other studies that use river-based measurements. A marked east-west gradient in simulated spring and summer DOC concentrations of 24 drainage basins on the North Slope of Alaska is captured by the modeling, consistent with independent data derived from river sampling. Nearly equivalent loading occurs to rivers which drain north to the Beaufort Sea and west to the Bering and Chukchi Seas. River basins on the North Slope are characterized by strong north-south spatial variations in runoff and DOC yield, with the former highest across the northern Brooks Range and the latter higher near the coast as influenced by abundant soil carbon stores. Significant increases in surface, subsurface (suprapermafrost), and total freshwater and DOC exports to Elson Lagoon in northwest Alaska are noted over the period 1981–2020. Our results show that increased DOC exports are attributable to warming soils and associated active-layer thickening. Indeed, direct

coastal suprapermafrost freshwater and DOC exports in late summer more than doubled between the first and last five years of the simulation period, with a large anomaly in September 2019 representing a more than fourfold increase over September coastal export during the early 1980s. These changes highlight the need for dedicated measurement programs and modeling studies that will enable improved understanding of climate change impacts on coastal zone processes in Arctic regions.

Plant Carbohydrate Depletion, Mycorrhizal Networks and Vulnerability to Drought: Experimental Tests in the Field

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Project: University Project
Project Website: N/A

Warming and drought associated with climate change are causing an increase in forest drought-induced mortality (DIM) around the world, which will have profound consequences from local to global scales. Predicting when, where and which trees will die of drought remains a challenge, in part, because the processes leading to DIM and their interactions are not fully understood. Empirical and modelling evidence indicate that most DIM occurs due to the interaction between impaired plant hydraulics and depletion of stored non-structural carbohydrates (NSC) under drought, but the mechanistic nature of this interaction is uncertain. Our prior work in the greenhouse showed that NSC storage depletion impairs plant water relations and that NSC depletion can spread through ectomycorrhizal networks. These results provide the opportunity to mechanistically quantify and model the interaction between NSC storage and plant hydraulics, and to incorporate symbiotic agents into DIM models via their effects on NSC storage and plant water relations. This project seeks to test in the field: 1) the mechanistic link between plant hydraulics and NSC storage, and 2) the potential for belowground fungal networks to affect this link and to influence forest vulnerability to drought. To this end, we are setting up a field experiment in *Pinus ponderosa* saplings, where we will manipulate carbon supply to the ectomycorrhizal network (EMN), water availability, and sapling connections to the EMN. During the fall of 2022 we set up 30 plots with three saplings each (**M**anipulated, to decrease carbon supply to the network; **R**esponse, to measure physiological responses; and **T**renched, to sever mycorrhizal connections and serve as a control). The perimeter of each plot has been trenched, and we covered half of the plots to minimize snow infiltration (drought treatment). We sampled soil around each sapling to identify common mycorrhizal species. Rain shelters will be installed later this month, and sapling manipulations and measurements will begin this spring. Our research addresses two challenges for modelling forest responses to drought: how to quantify and model the interdependency between plant hydraulics and carbohydrate availability, and how to incorporate interactions with belowground symbiotic organisms.

Tropical trees as Conduits for Connecting Belowground Microbial Processes to Aboveground Methane Emissions at the Terrestrial Aquatic Interface

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BER Program: ESS
Project: University project

Our project investigates the influence of trees on methane emissions from both flooded (varzea) and *terra firme* forest sites along the Amazon river near Santarem, Brazil. In our first year we (1) identified a site for the flooded forest tower (east of the community of Pixuna across the Amazon river from Santarem); (2) ordered tower parts and instruments for the tower for eddy covariance measurements of methane, carbon dioxide, water and energy; (3) equipped the *terra firme* tower for initial methane flux measurements (started this rainy season with borrowed equipment from AmeriFlux); (4) mentored honors college undergraduate engineering students to design and test chambers for soil/water and tree stem flux system for the flooded site; (5) made initial manual measurements of soil and tree stem fluxes and sampled soil microbial communities in the dry and wet season, and (6) engaged with media liaisons and graduate students from the ASU Cronkite center to document the science process through photo and video shoots and interviews. Initial measurements with the new Licor 7810 (portable CH_4, CO_2, H_2O analyzer) in the dry season/start wet season demonstrated that tree stem methane fluxes were ~10 times larger in the varzea site than the upland site ($63.5_{27.9}^{49.}$ vs $6.0_{2.9}^{4.9}$ μg-C m^{-2} h^{-1} respectively; t-test $P<0.0001$), whereas stem carbon dioxide fluxes were only marginally significantly different between the sites (varzea 163±34 vs upland forest 114±35 mg-C m^{-2} h^{-1}; t-test $P=0.04$). Stem methane fluxes in the dry season appeared to be related to stem wood density with trees with higher wood density showing lower fluxes. Dry season soil fluxes at the upland forest showed mainly methane consumption whereas the varzea sites had mainly methane production (-27_{15}^{19} vs 59_{42}^{58} μg-C m^{-2} h^{-1}, respectively; t-test $P<0.0001$). Soil carbon dioxide fluxes were only marginally different between sites (varzea 271±113 vs upland forest 170±30 mg-C m^{-2} h^{-1}; t-test $P=0.08$). We will discuss these results also in light of the microbial communities as that data becomes available. The next step will be to measure the stem and soil fluxes in the wet season, in late May, when the varzea site will go through the maximum flooding stage.

Title: Influence of Hyporheic Exchange on Coupled S-Fe-C biogeochemical cycling and Microbial Community Function in Riparian Wetlands at the Savannah River Site

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Project Lead Principal Investigator (PI): Cara Santelli

BER Program: ESS

Project: University Project

Project Abstract: Riparian wetland hyporheic zones where oxic surface water and anoxic groundwater mix, drive steep redox gradients and promote hotspots and hot-moments of biogeochemical processes. In freshwater wetland and stream sediments, carbon (C) turnover and fate is heavily influenced by the biogeochemical cycling of iron (Fe). "Hidden" or "cryptic" sulfur (S) redox processes may be further coupled to these Fe and C cycles. S biogeochemical cycling is not well constrained in freshwater systems but can include the production of reactive intermediate S species that promote further biotic and abiotic redox reactions (including those coupled with Fe reduction and methane oxidation), thus supporting higher rates of sulfur biogeochemical cycling than otherwise expected in these low sulfate environments. The overall goal of this project is to develop a mechanistic understanding of how hydrologic flow influences coupled abiotic-biotic Fe-S-methane cycles in riparian wetlands.

In the uncontaminated area of Tims Branch at the Savannah River Site, we set up several sites with continuous surface- and ground-water level and flux measurements and seasonal sampling of water and sediments. Specifically, we examined the primary Tims Branch stream, a hydrologically dynamic stream tributary containing Fe oxide-encrusted microbial mats or "Fe flocs", a large wetland with abundant "Fe flocs", and a small sulfide-enriched pond of water connected to the wetland. Microbiome analyses revealed the microbial community was highly similar between sites regardless of season, except for changes in the relative abundance of phyla with depth. Quantitative PCR revealed that both dissimilatory sulfite reduction (dsr) and adenylylsulfate reductase (apr) genes were enriched in gaining stream sites (e.g., wetland, tributary), indicating that sulfate reduction is an important process despite relatively low sulfate levels and below-detection porewater sulfide concentrations. In support of a cryptic sulfur cycle, shotgun metagenome sequencing revealed a greater abundance of sulfur oxidation and thiosulfate oxidation genes in anoxic sediments in the gaining environments relative to the primary losing stream. Despite the reduction environment, porewater geochemical analysis measured high aqueous or colloidal Fe(III) concentrations, which could fuel this cryptic S cycle.

Title: **WATERSHED CONTROLS ON URANIUM CONCENTRATIONS TIED INTO NATURAL ORGANIC MATTER AND IRON INTERACTIONS IN STREAMBEDS AND WETLANDS**

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Project Lead Principal Investigator (PI): Peter H. Santschi

BER Program: EES

Project: **Collaborative Research: Watershed Controls On Uranium Concentrations Tied To Natural Organic Matter In Streambeds And Wetlands**

Project Abstract:

To address this hypothesis, we are first addressing the following set of questions through field-oriented studies at the Argonne Wetland Hydrobiogeochemistry SFA field site (a U-contaminated wetland of the Savannah River Site) and accompanying laboratory experiments: 1) What is the optimal method(s) to differentially extract stable (immobile) versus mobile natural organic matter (NOM) from the same sedimentary or aquatic sample? We developed a method capable of differentially extracting immobile and mobile NOM fractions (high-molecular-weight and low-molecular-weight components for each) that are suitable for molecular-level chemical characterization via Fourier-transform ion cyclotron resonance mass spectrometry (FTICR-MS). 2) How does NOM composition impact the physical properties (e.g., hydrophobicity) underlying their aggregation/disaggregation behavior? How do diagenetic processes affect the massive occurrence of flocs in the gaining stream and the scavenging of U? We observed NOM concentrations (as calculated as the sum of carbohydrates and proteins in mg-NOM/g-particles) increasing in the order of floc > suspended particulate matter (SPM) > bottom sediment; whereas, the protein-to-carbohydrate ratio (an index for stickiness for aggregation) was in the order of SPM > flocs > bottom sediment. Flocs contained 4 to 5-fold higher U than the stream bottom sediment. 3) What is U distribution in a dynamic watershed with relevance to groundwater-surface exchange? 4) What role does sedimentary phosphorus speciation play in U distribution in this watershed? Information from this project will identify and quantify important hydrologically driven biogeochemical processes impacting uranium at this SFA.

Title: Developing a probabilistic framework to capture redox heterogeneity and greenhouse gas predictions in Terrestrial-Aquatic Interfaces

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Project Lead Principal Investigator (PI): Debjani Sihi
BER Program: Environmental System Science (ESS)
Project: University project (DE-FOA-0002392)
Project Website: https://ess.science.energy.gov/summary-of-environmental-system-science-projects-awarded-in-summer-2021/

Project Abstract: Terrestrial-Aquatic Interfaces (TAIs) represent dynamic transition zones between land and water, where steep physical, chemical, and biological gradients converge for accelerated biogeochemical transformations and greenhouse gas (GHG) emissions. Hydrological dynamics strongly affect redox conditions that drive the transformations of redox-sensitive elements such as nitrogen (N), dissolved organic matter (DOM), iron (Fe), manganese (Mn), and sulfur (S). These transformations impact soil organic matter (SOM) decomposition and GHG emissions. Currently, these complex interconnected processes remain underrepresented in ecosystem and Earth system models (ESMs) because we lack modeling tools that can directly constrain and parameterize heterogeneity in redox processes that vary at highly condensed spatial and temporal scales. To address this gap, we are building a dynamic modeling framework that captures the heterogeneity at microsite-scales, which drives hot spots and hot moments of GHG emissions at ecosystem scales across TAIs. We leverage probability density functions (PDFs) to capture numerically the spatiotemporal heterogeneity of soil microsites needed to predict non-normal distributions of microbial activity. We hypothesize that modeling of plot-scale and ecosystem-scale dynamics of GHGs can be improved by integrating and upscaling microbial metabolic activities at the microsite-scale. Our new modeling framework (Redox-DAMM) merges the capabilities of microsite PDFs of the DAMM-GHG model (Dual Arrhenius and Michaelis Menten-GreenHouse Gas, Sihi et al., 2020, Global Change Biology, DOI: 10.1111/gcb.14855) with a redox reaction network model (Zheng et al., 2019, Biogeosciences, DOI: 10.5194/bg-16-663-2019). The Redox-DAMM framework contains three key components: (1) Microsite PDFs, (2) PDF-constrained redox reaction networks, and (3) Redox reaction networks within the soil pore-network that inform diffusion-limitation of substrates related to the production and consumption of GHGs. Soil heterogeneity represents an important, yet unresolved, component in biogeochemical models. We will demonstrate that dynamic representations of redox heterogeneity improve model performance of GHG emissions in TAIs. Microsite PDF function-based computational tools represent a great advance in generating transferrable modeling capability from fine-scale processes to ecosystem-scale functions, directly supporting BER priorities of understanding multi-scale Earth system dynamics and processes.

Title: Tidal Wetland Flux Network: Plans and Progress

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Project Lead Principal Investigator (PI): Patty Oikawa, Lisamarie Windham-Myers

BER Program: Environmental System Science

Project: University project

Project Abstract:

Abstracts should include information on objectives of the research, recent progress, and key findings of the project

High-frequency Data Integration for Landscape Model Calibration of Carbon Fluxes Across Diverse Tidal Marshes

We aim to improve understanding and assist process-based modeling of ecosystem-scale gross primary productivity (GPP) and CH4 fluxes. Using a network of seven eddy covariance flux tower sites, we will investigate both nonlinear and asynchronous responses to stressors including plant inundation, disturbance, salinity, and nitrogen loading in tidal wetlands at the tidal aquatic interface.

Effect of Hydrological Forcing on the Biogeochemical Transformation of Carbon and Greenhouse Gas Emissions in Riparian and Streambed Sediments

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BER Program: ESS

Project: University project

Project Abstract: Biogeochemical processes in riparian and hyporheic sediments regulate the transformation and exchange of carbon, nutrients, and greenhouse gases (GHGs) with surface waters. Riparian and hyporheic zones are terrestrial-aquatic interfaces (TAIs) where hydrological processes create strong biogeochemical gradients and redox microniches that are metabolically highly variable and influenced by temporal variations in precipitation, temperature, and stream discharge. The complex temporal and spatial variability of hydrological variations in riparian and hyporheic sediments create hot spots and moments that are difficult to quantify and account for in reactive transport models (RTMs). In addition, reactive transport in these systems is traditionally simulated on the continuum scale using upscaled empirical parameters that are not able to reproduce the effect of biogeochemical reactions on pore scale heterogeneities and their feedback on biogeochemical rates. These effects tend to overestimate rates at the Darcy scale and misrepresent GHG emissions from riparian and streambed sediments. In this new project, state-of-the-art in situ physical and geochemical measurements with high spatiotemporal resolution will be combined with meta-omic signals of the active microbial populations in riparian and hyporheic sediments of Steed Pond at the Savannah River National Laboratory to: 1) predict the role of hydrological forcing on the spatiotemporal transformation of carbon, nutrients, and redox processes along this gaining and losing wetland stream; and 2) determine the effect of these hydrobiogeochemical processes on GHG emissions. Gene-centric microbial metabolic rate laws developed during a previous exploratory project are currently integrated in pore-scale and continuum RTMs that will be combined with machine-learning algorithms to assess model sensitivity and calculate biogeochemical rates. Characterizing the distribution of the main redox species in wetland and stream sediments with high spatial and temporal resolution will provide unique insights into the processes that control GHG emissions from riparian and streambed sediments under varying hydrological conditions. The newly developed numerical models will predict how variations in hydrological forcing, competition between microbial metabolic processes, and porosity changes associated with biogeochemical feedback affect carbon and nutrient cycling as well as GHG emissions at TAIs. Ultimately, these efforts will capture the role of sediment heterogeneities in GHG emissions.

Applying "R-Osmos" To Quantify Hot-Moments in a High Mountain Watershed: Co-Development of Novel Methodology To Advance Terrestrial-Aquatic Interface Models

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BER Program:ESS

Project: University Project

Project Abstract: Watershed function is driven by habitat heterogeneity and microbial activity integrated over space and time. These habitats experience seasonal changes in redox zonation with water flow shifting biogeochemical cycles and perturbing the microbial communities that mediate biogeochemical processes. Features such as river meanders can create hot spots of biological activity, however they must be directly sampled to be understood. This newly funded project will quantify the impact of hot spots and moments on microbial rates, focusing on two critical processes: methane (CH_4) oxidation and nitrate (NO_3) reduction, at the DOE's East River Watershed Function Science Focus Area. We will deploy novel, continuous, time-integrating, *in-situ* microbial rate samplers to inform the magnitude and variation in biogeochemical processes across the terrestrial-aquatic interface, which upon completion, will be used to refine a reactive transport model for this area. To accomplish this goal, we will use uniquely configured osmotic samplers (OsmoSamplers) to continuously quantify the rate at which microbial communities transform methane and nitrate on either side of a meander. OsmoSamplers use a diffusion gradient to slowly pump water into tubes of such small diameter that sample mixing is negated. Multiple OsmoSamplers can be used together to continuously add solutes, preservatives, or collect samples for later analysis, providing a record of hot moments in long-term datasets. In this work, we will use rate-osmotic samplers (R-osmos) to acquire spatially explicit rate measurements by adding nitrate and methane (separately) to discern transformation of these critical compounds. Rates will be coupled with quantifications of natural solute composition (both NO_3 and CH_4) and quantitative gene abundance for the relevant processes (i.e., genes responsible for nitrate reductase and methane monooxygenase) allowing us to connect solute, rate, and microbiome characteristics. This project was recently initiated, with the majority of the work thus far being preparation for our planned year-long field deployment that will commence in summer 2022. In this presentation, we will cover the overall aims of the project, update progress to date, and highlight opportunities that this research framework may provide for collaboration with other SFA users.

In-situ Observations of Organic Carbon Oxidation in Shale Regolith and Implications for Bedrock Weathering

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Project Lead Principal Investigator (PI): Jennifer L. Druhan

BER Program: ESS

Project: University project

Project Abstract:

Oxidation of organic carbon hosted in bedrock (petrogenic OC, OC_{petro}) is increasingly recognized as a source of CO_2 to the atmosphere on century and millennium timescales as sedimentary bedrock is exposed to oxidizing conditions through uplift, channel incision, and erosion. Recent studies point towards the near-surface as a region of enhanced OC_{petro} oxidative weathering in watersheds. However, we do not know how the exposure of OC_{petro} in bedrock to this dynamic, oxidative, and vegetated environment affects the rates of OC_{petro} oxidation along the gradient of environmental conditions that exist within the near-surface weathering profile. Here, we use specialized in-situ samplers distributed throughout a shale weathering profile to determine the rate of OC_{petro} oxidation at the same location where significant respiration rates have been documented in weathered bedrock. The 16 m deep argillaceous weathering profile is located along a steep, rapidly eroding hillslope in the Northern California Coast Ranges, where deep tree roots seasonally withdraw water from depths of up to 12 m. CO_2 production within the deep root zone in bedrock constitutes between 2 and 29% of the total flux of CO_2 from the ground surface. Chemical depletion of OC_{petro} in the solid phase beneath the root zone where no modern OC was present in the solid shows that OC_{petro} is removed from weathered bedrock at a rate of 0.12 gC/m^3/year. This rate is much smaller than the 557.1 gC/m^3/year oxidation rate of OC_{petro} from lab incubations, indicating significant controls that limit the full oxidation of OC_{petro} in the weathering profile. In addition, radiocarbon analyses of the gas phase are entirely modern to 15 m, undermining the ability to determine the amount of removed OC_{petro} that is oxidized within the weathered bedrock profile. These results highlight the importance of investigating the controls on respiration of recently photosynthesized OC. This study finds that recently fixed carbon dominates respiration in a weathered bedrock profile where roots are deep, masking any potential OC_{petro} oxidation at the rates at which it is removed from the solid phase, and pointing towards further avenues of study to understand the limitations on OC_{petro} oxidation.

Title: **Effects of ecohydrological patches on methane emissions and carbon sequestration in coastal wetlands**

Jorge Villa[1,*], Yang Ju[2], Theresia Yazbeck[2], Robert Bordelon[1], Djennyfer Ferreira[3], Diana Taj[1], Sergio Merino[4], Eric Ward[4], William Riley[5], Kelly Wrighton[3], Gil Bohrer[2]

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Project Lead Principal Investigator (PI): Gil Bohrer

BER Program: ESS

Project: University Project (DE-SC0021067) – Functional-type modeling approach and data-driven parameterization of methane emissions in wetlands

Project Abstract: Methane emissions from coastal wetlands represent an important portion of the global greenhouse gas budgets. Coastal wetland experience increasing disturbance rates associated with changes to hydrology, sea level, and climate. At our Ohio wetland site, OWC, long term water level rise of Lake Erie (~1 m in the last decade) provides drive changes to the wetland's ecology, and as OWC gets deeper, mudflats and cattails give way to open water and floating-leaf vegetation.

We conduct chamber-based patch-level measurements and site-scale eddy covariance measurements of methane and carbon fluxes at the wetland sites. Our observations quantify the ecological and physical differences that lead to very large differences in flux rates at different eco-hydrological patch types. We used soil cores a long depth transects at areas of the wetland with different hydrological regimes to study the relationships between carbon and nutrient sequestration at different areas of the wetland. We developed an approach to classify the eco-hydrological patch type from remote sensing images. We used seasonal time series of NDVI from HLS (a composite dataset of Sentinel and Landsat) to develop a decadal map of patch type locations and extent at our Ohio wetland.

Our observations represent a valuable foundation towards a more robust models of methane fluxes in wetlands at the resolution of within-wetland vegetation patch type and resolving the effects of seasonal and within-season vegetation phenology in ecosystem-scale models. We are currently working on implementing insight from our observations in an advance version of E3SM-ELM that treats wetlands as land units and resolves within-wetland patch functional types.

Title: **Influx of Oxidants into Reduced Zones: Microbiological Controls Governing Metal Oxidation and Reduction**

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Project Lead Principal Investigator (PI): Karrie A. Weber
BER Program: ESS
Project: University led project
Project Website: NA
Project Abstract:
The existing paradigm describes oxidation of reduced chemical species, such as iron(II) and uranium(IV), following an influx of oxidants such as dissolved oxygen (DO) or nitrate. Prior field results challenged current understanding of the oxidant's role controlling redox behavior of metals/radionuclides; low concentrations of an oxidant (DO) injected into a biostimulated reduced region of an alluvial aquifer stimulated a decrease in aqueous uranium concentrations *in situ* [1]. Here we experimentally test the impact of a highly soluble oxidant, nitrate, on metal/radionuclide redox state using organic-rich, naturally reduced-uranium bearing oxbow lake sediments. Batch reactors of reduced sediments preincubated with uranyl chloride as a redox tracer were amended with and without the addition nitrate at varying concentrations (low nitrate <14 mg/L-N> high nitrate). High nitrate amended batch reactors increased dissolved uranium(VI) consistent with oxidation of reduced species. However, low nitrate amendments stimulated a decrease in dissolved uranium(VI), consistent with reduction. No significant change was observed in reactors amended with anoxic deionized water. X-Ray Absorption Near Edge Spectroscopy analysis of sediments supported uranium(VI) reduction with the precipitation of uranium(IV). An increase in aqueous iron(II) further supported the onset of reducing conditions. Reduction activity occurred concurrent with an increase in dissolved organic carbon (DOC) and cell and virus abundance. Batch reactors were amended with the antibiotic chloramphenicol demonstrated suppression of nitrate and uranium reduction supporting this as a microbially catalyzed process. Metagenome assembled genomes from the microbial community revealed the metabolic potential indicating complex carbon degradation, fermentation, mineralization as well as the potential for anaerobic respiration of nitrate, metal/radionuclides, and sulfate. Recovery of metagenome assembled virus genomes from microbial (>0.2μm) and virome (<0.2 μm and >0.05 μm) samples indicated a change in viral community in response to nitrate amendments as well as viral-encoded carbohydrate active enzymes suggesting a microbial and viral liberated carbon. Together these results indicate that an influx of an oxidant can lead to the increase in DOC and carbon cycling supporting microbial activity and reducing conditions below a nitrate threshold or "tipping point".

[1] Pan et al., *Environ. Sci. Technol*. 2018. 52: 8133–8145.

Title: **Integrating data and models to enhance our understanding of the effects and drivers of shrub encroachment in US tallgrass prairie**

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Project Lead Principal Investigator (PI): Jesse Nippert

BER Program: TES

Project: DE-SC0019037

Project Website: NA

Project Abstract: Shrubs are encroaching upon and eradicating many grasslands across Earth, and we currently have very limited understanding about (1) why this is occurring, and (2) the resulting consequences for critical ecosystem services, such as carbon sequestration. Our project is designed to address both of these knowledge gaps through a combination of observational, experimental, and process-based modeling approaches in tallgrass prairie of eastern Kansas. More specifically, we have measured a wide range of above and belowground morphological and physiological characteristics of shrubs and grasses, as well as soil carbon turnover rates within the grass-shrub ecotone; we imposed a multi-year drought experiment to understand responses of grasses, shrubs, and carbon cycling to water stress; we are incorporating this empirical understanding into process-based models to test hypotheses about why shrub encroachment is occuring and to project impacts of encroachment on ecosystem carbon storage. In this Spark presentation, we will show findings associated with each of these approaches. Briefly, we found that shrubs had lower photosynthetic rates than grasses, but photosynthesis was more stable under drought, likely due to smaller yet more numerous conduits in roots. Instead of the expected increases in carbon storage by shrubs in deeper soils, we found less carbon storage across all depths under shrubs as well as carbon loss shrubs that have recently encroached on grasslands. By incorporating our empirical data into CLM-FATES and BiomeE, we are able to recreate historical (1983-current) patterns of shrub encroachment at our field site. We are using these models to test multiple drought-related mechanisms behind shrub encroachment, and find that drought events provide shrubs a foothold to advance into grass-dominated areas. Our initial model projections suggest that the consequences of shrub encroachment include a decadal reduction in soil carbon storage for these grasslands and that reversal back to grassland states is

difficult to achieve once shrub encroachment has occurred. In total, these findings highlight the importance of maintaining these grasslands into the future, especially as they are difficult to recover after being lost.

Title: **Impacts of streambed dynamics on nutrient and fine sediment transport in mountain rivers**

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Project Lead Principal Investigator (PI): Elowyn Yager

BER Program: ESS

Project: University Project

Project Abstract: In mountainous watersheds, rivers typically have an armor layer of coarse sediment that protects the finer subsurface from erosion. In theory, armor layer motion during high magnitude flows could release the subsurface fine sediments that are often enriched in Phosphorus (P) and Particulate Organic Carbon (POC). Hysteresis and seasonal variations in POC, soluble reactive phosphorus (SRP), particulate phosphorus (PP), and suspended sediment (SS) may therefore be partly controlled by armor layer motion. In addition, streambed concentrations of these constituents may depend on whether a reach is losing or gaining. We are currently testing whether armor layer motion and streambed concentrations influence hysteresis patterns during summer monsoon and snowmelt seasons in one gaining and one losing reach of La Jara Creek in Valles Caldera National Preserve, NM. We are measuring armor layer motion, streambed and river concentrations of POC, PP, SRP, and fine sediment as well as surface and groundwater exchange in these two reaches. In addition, we are conducting field experiments that isolate the effects of armor layer removal on nutrient and fine sediment concentrations in the water column. Preliminary results demonstrate generally similar hysteresis patterns of PP, SRP and fine sediment in one monsoon driven event that moved the armor layer. The final results of this work will determine how perturbations, such as the sequence and magnitude of droughts and floods, constrain biogeochemical nutrient cycling and impact subsequent temporal variations in nutrient and fine sediment export from mountainous watersheds.

Title: **Biophysical Processes and Feedback Mechanisms Controlling the Methane Budget of an Amazonian Peatland**

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BER Program: Terrestrial Ecosystem Sciences (TES)
Project: University Project Award Number DE-SC0020167
Project Website: https://biometeorology.umn.edu/research/quistococha-forest-reserve-qfr-amazonian-ameriflux-site-iquitos-peru

Project Abstract:

Tropical peatlands are one of the largest natural sources of atmospheric methane and are keystone ecosystems that play a significant role in regional and global carbon budgets. However, we have a poor understanding of how these ecosystems function and respond to climate variability leading to large uncertainties of their carbon cycle processes and budgets. In addition to the scarcity of tropical peatland observations, another challenge is how to mechanistically describe the complexity of biogeochemical processes in ecosystem models. Based upon the measurements at an eddy covariance flux site established in a tropical palm swamp peatland near Iquitos, Peru, this project seeks to understand the biophysical controls on carbon cycle processes in tropical peatlands, and to advance the predictive capability of DOE's E3SM land model (ELM) for the carbon budget.

Over the past year our team has conducted research focused on the following project objectives: **(a) Partitioning net ecosystem carbon fluxes and quantifying soil and stem carbon fluxes associated with varying microtopography and dominant tree species.** Average soil CO_2 and

CH_4 fluxes were 0.55±0.04 μmol m^{-2} s^{-1} and 16.06±0.86 nmol m^{-2} s^{-1} respectively. Average stem CO_2 fluxes from *M. flexuosa*, *M. aculeata,* and *T. insignis* were 0.06±0.01, 0.10±0.01, and 0.20±0.01 μmol m^{-2} s^{-1}, respectively, and average CH_4 fluxes were 0.23±0.15, 0.39±0.11, and 0.07±0.18 nmol m^{-2} s^{-1}, respectively. Our preliminary results during wet seasons indicate that there are no significant dial patterns or spatial heterogeneity for both soil and stem carbon fluxes. **(b) Applying satellite remote sensing observations to investigate the spatiotemporal patterns of vegetation productivity in the broader Pastaza-Marañón peatland basin.** This work incorporates high-resolution land cover data, sun-induced chlorophyll fluorescence and we are now working to bring in near-infrared reflectance from vegetation into the analysis to better match the spatial resolution of the land cover data. A major goal is to test for differences among vegetation types, specifically forests growing on peatland vs. mineral soil. **(c) Improving the ELM model for tropical peatlands.** We have identified the important controls of vegetation processes on the carbon budget in the Amazonian swamp peatland and found that different carbon feedbacks to warming and drought conditions exist in tropical and boreal peatlands. Together, our measurement and model results highlighted the unique properties of carbon flux components and the importance of vegetation (i.e. stomatal regulation, nitrogen-photosynthesis relationship, and phenology) and soil microbial (i.e. acetoclastic methanogens) processes for carbon cycling in the tropical swamp peatland.

Title: Seasonal Hydrologic Forcings Drive Salt Marsh Function

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Project Lead Principal Investigator (PI): Margaret Zimmer

BER Program: ESS

Project: University Award (DE-FOA-000218)

Project Website: http://mzimmer.weebly.com/nitrates.html

Project Abstract:

Salt marshes exist at the terrestrial-aquatic interface (TAI) between watersheds and the ocean. These tidal systems are hot spots of biogeochemical activity, yet we have limited understanding of their hot moments, or temporal dynamics of nutrient processing. Specifically, we have limited understanding of how daily tidal cycles and seasonal terrestrial water inputs (e.g., seasonally elevated groundwater) interact within these TAIs to drive biogeochemical processing in the subsurface. To address this knowledge gap, we instrumented a 25 m transect along a representative salt marsh platform at the Elkhorn Slough National Estuarine Research Reserve in California, USA. We installed variable-depth redox probes, nested piezometers, and a field-deployable spectrophotometer with a multi-source pump at lower, mid, and upper marsh positions to allow for characterization of subsurface hydrologic cycling and biogeochemical behavior at a high frequency (~15 min). We also conducted seasonal sediment incubation experiments to quantify nitrogen processing rates as well as monthly vegetation surveys, monthly pore water sampling campaigns, and subsurface sediment characterization (e.g., porosity, texture, organic matter). Finally, we paired these observations with measurements of terrestrial groundwater dynamics in adjacent uplands with tidal surface water monitoring to understand potential water inputs into the marsh through time. We found that biogeochemical behavior ranged as a function of time-scale. Dissolved inorganic nitrogen concentrations fluctuated hourly due to frequent tidal flushing that introduced oxygen and ammonium-rich surface water into sediments under reduced conditions, with the largest change in concentrations observed in lower marsh positions. Sediment core incubations showed a dominance of net N_2 flux out of the marsh, indicating removal by denitrification. However, we identified that the impacts of seasonal and event-driven freshwater contributions affected the biogeochemical

behavior of marsh elevations differently, with the largest changes seen in upper marsh positions. Together, our findings suggest that intra-annual changes in source water contributions across the marsh result in functional zonation, where lower marsh position functions may be regulated by tidal flushing and upper marsh position functions may be regulated by freshwater contributions.

Title: **ML-enabled assimilation of community geochemical datasets into reactive transport models**

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BER Program: ESS

Project: DOE Lab-led project

Project Abstract:

Laboratory experiments are critical to interrogate the impact of hydrological and climate perturbations on biogeochemical (BGC) processes in a controlled environment. Hydrologically driven biogeochemical reactions are a key aspect of the Earth system predictability, particularly at dynamic interfaces (e.g., terrestrial-aquatic interfaces, hot spots), governing the cycling of nutrients, metals, and organic matter. Recently, there has been a significant effort to collect and compile relevant experimental data across the community, and to develop machine-readable experimental databases for various elements and species in different conditions. Developing such large database has created a unique opportunity for machine learning (ML) to gain new scientific insights as well as to improve the parameterization and uncertainty quantification within BGC and reactive transport models (RTMs).

In this project, we develop an ML-enabled paradigm shift to integrate laboratory experiments and their data into a framework for subsequent incorporation into Earth Systems models with the FAIR (findability, accessibility, interoperability, and reusability) principle. In particular, we aim to a) establish the experiment-to-simulation pipeline through an open-source python/R suite of codes, (b) develop various unsupervised and supervised learning capabilities coupled with the database, and (c) characterize the parameter and model uncertainties across the global datasets in the Bayesian method and transfer the uncertainty to simulation results in a seamless manner.

During the course of our project, the team has developed a new workflow to govern experiment-to-simulation pipelines initially focused on surface complexation reactions, and has also released the accompanying python/R scripts to the public under LLNL distribution.[1] Additionally, we are developing a high-performing, hybrid ML model informed by the chemical thermodynamic

[1] https://ipo.llnl.gov/technologies/software/llnl-surface-complexation-database-converter-scdc

principles.[2] This new approach exploits the previous FAIR-based database development work and paves the way for a more nuanced perspective between traditional sorption modeling routines and pure ML methods. In parallel, a new Python-based workflow has been developed to quantify parameter and model uncertainties associated with PHREEQC-based geochemical simulations using Bayesian methods. Lastly, we are using this pipeline in the development of a watershed reactive transport model for simulating weathering and ion exchange processes. The work is intended to be general and extensible to other BGC data, and to provide a framework for their implementation in discovery science and Earth Systems modeling. In addition, we envision that this framework will stimulate the developments of other community-wide experimental database in BGC and beyond.

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From tides to seasons: How cyclic tidal drivers and plant physiology interact to affect carbon cycling at the terrestrial-estuarine boundary

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BER Program: ESS

Project: Other Institution project

Project Website:

Project Abstract: Our overarching goal is to improve mechanistic process understanding and modeling of tidal wetland hydro-biogeochemistry in coastal Terrestrial-Aquatic Interfaces. Key characteristics that distinguish coastal wetlands, such as tidal oscillation, sulfur biogeochemistry, and plant structural adaptations to anaerobic soil, are beginning to be incorporated in land surface models such as the E3SM Land Model (ELM) through coupling with reactive transport code (ELM-PFLOTRAN). There remains large uncertainty in their parameterization. Particularly challenging are: 1) the small-scale, dynamic, heterogeneous redox conditions in wetland soils; 2) the aerenchyma tissue in wetland plants that greatly facilitate gas fluxes into and out of sediment; and 3) the temporal and spatial variability in salinity, which is a key determinant for plant species distribution and productivity, as well as organic matter decomposition.

Working in a brackish marsh, we will combine intensive and new spatially-explicit sediment redox measurements with continuous sediment redox, salinity, and water table data, and then test relationships between these sediment variables and atmospheric fluxes of carbon and energy. Measurements will be guided by, and will inform, new developments in ELM-PFLOTRAN designed to capture critical features of diverse coastal TAI functions. We plan integrated measurements and modeling at two locations with contrasting hydro-biogeochemistry in an oligohaline marsh in the Parker River estuary, MA. We will use field measurements to help inform ELM-PFLOTRAN development designed to improve simulations of brackish marsh biogeochemistry under fluctuating oxygen availability and salinity influenced by tides, diel and seasonal changes in plant physiology and river discharge.

Ultimately, we will be poised to combine our new process understanding and model formulation with existing long-term data already in hand from two more saline salt marsh sites in the Parker Estuary. As sea level rises, saline conditions will become more common in many coastal TAIs, but they will also potentially be exposed to more flashy freshwater riverine input from intense, sporadic, storms. By having information from marshes at both ends of the full salinity gradient, we will be able to better constrain biogeochemical reactions in ELM-PFLOTRAN, validate ecosystem-scale modeled fluxes with eddy covariance measurements, and simulate present and

future hydrological variations and resulting carbon dioxide and methane fluxes in tidal wetlands in the face of expected global change.

Title: **Catastrophic Forest Disturbance and Subsequent Regrowth in Puerto Rico Following Hurricane Maria**

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BER Program: ESS
Project: Other Institution project

Project Abstract: Tropical cyclonic storms are an important cause of forest disturbance in coastal zones. We analyzed data from high density airborne lidar from Puerto Rico collected prior to Hurricane Maria (2017) and about eight months (2018) and 30 months (2020) following the storm. Our analyses covered both an elevational gradient (439 ha) from 100 to 800 m ASL in the El Yunque National Forest and transects (25,188 ha) distributed across the island. On the elevational transect, we found that forest canopy damage was widespread, with 73% of the study area losing ≥1 m in canopy height (mean = -7.1 m). Taller forests at lower elevations suffered more damage than shorter forests above 600 m. Yet only 13.5% of the study area had canopy heights ≤2 m after the storm in 2018 highlighting the importance of damaged trees and advanced regeneration on post-storm forest structure. Heterogeneous patterns of regrowth and recruitment yielded shorter and more open forests by 2020. Nearly 45% of forests experienced initial height loss >1 m (2017-2018) followed by rapid height gain >1 m (2018-2020), whereas 21.6% of forests with initial height losses showed little or no height gain, and 17.8% of forests exhibited no height changes larger than ±1 m in either period. Canopy layers <10 m tall accounted for most increases in canopy height and fractional cover between 2018-2020, with gains split evenly between height growth and lateral crown expansion by surviving individuals. Across the island of Puerto Rico, we measured canopy damage using flights from 2017 and 2018. Island-wide, canopy height decreased by an average of 4.8 m, or 34%, from a mean height of 13.2 ± 6.1 m before the storm to 8.4 ± 4.1 m after the storm. We selected 140,000 grid cells randomly from our full lidar collection (370,885 grid cells) stratified on estimated peak wind speed (Tropical storm, Category 1, or Category 2) and forest type (wet, moist, and dry). Using a Random Forests analysis, we found that the absolute change in canopy height was best predicted by pre-storm canopy height, maximum sustained wind speeds, and the distance from the path of the storm. We seek to understand how these data can be used to calibrate and benchmark FATES and other models. Our data inform rates of gap formation, crown expansion, and canopy closure following hurricane damage and highlight the diversity of ecosystem impacts from heterogeneous spatial patterns and vertical stratification of forest regrowth following a major disturbance event.