

# 2024 Environmental System Science PI Meeting Abstracts

# April 16–17, 2024

U.S. Department of Energy Office of Science Biological and Environmental Research Program Earth and Environmental Systems Sciences Division



Biological and Environmental Research Program

# 2024 Environmental System Science PI Meeting

# April 16-17, 2024

## **Reston**, Virginia

U.S. Department of Energy Biological and Environmental Research Program (BER) Earth and Environmental Systems Sciences Division (EESSD)

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The Biological and Environmental Research (BER) program supports transformative science and scientific user facilities examining complex biological, Earth, and environmental systems for clean energy and climate innovation. BER research seeks to understand the fundamental biological, biogeochemical, and physical principles needed to predict a continuum of processes occurring across scales, from molecules and genomes at the smallest scales to environmental and Earth system change at the largest scales. This research—conducted at universities, U.S. Department of Energy national laboratories, and research institutions across the country—is contributing to a future of reliable, resilient energy sources and evidence-based climate solutions.

#### **About ESS**

The Environmental System Science (ESS) program advances an integrated, robust, and scale-aware predictive understanding of terrestrial systems and their interdependent biological, chemical, ecological, hydrological, and physical processes. ESS is part of the Earth and Environmental Systems Sciences Division within the U.S. Department of Energy's Biological and Environmental Research Program. ESS activity seeks to develop an integrated framework using a systems approach to elucidate the complex processes and controls on the structure, function, feedbacks, and dynamics of terrestrial ecosystems that span from the bedrock through the rhizosphere and vegetation to the atmospheric interface.

This abstract book is available at ess.science.energy.gov/pi-meeting/

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Biological and Environmental Research Program

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# Terrestrial Ecology

Terrestrial ecology research supported by the Environmental System Science program seeks to improve the representation of terrestrial ecosystem processes in Earth system models, thereby enhancing the robustness of model projections and providing the scientific foundation for solutions to the U.S. Department of Energy's most pressing energy and environmental challenges.

# Terrestrial Ecology University Projects

# Rhizodeposition and the Fate of Mineral-Associated Soil Carbon

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Mineral-associated organic matter (MAOM) is a dominant component of total soil carbon (C). Once bound to reactive soil minerals that organic matter can be protected for millennia. Individual compounds commonly released by roots can mobilize MAOM off minerals to different extents, via different mechanisms, making the OM vulnerable to microbial attack. Carbon dioxide  $(CO_2)$  can then be released, and nutrients can be moved back into rapidly cycling pools, potentially creating a feedback to plant root activity. But rhizodeposits from living roots are complex mixes of compounds, and their quality and quantity vary with environmental conditions., Beyond demonstrating that individual compounds commonly lost by roots have the potential to mobilize MAOM, taking the next step requires exploring how naturally complex and dynamic mixes of rhizodeposits from live roots affect MAOM pool dynamics in soil. Researchers conducted two greenhouse growth chamber experiments quantifying the capacity of live root systems to mobilize MAOM off minerals as a function of altered morphology and physiology triggered by Barley Yellow Dwarf Virus (BYDV) infection, as a function of low soil nutrient and water availability. Among other results, respiration

from soil under BYDV-infected plants had a higher percent <sup>13</sup>C-MAOM-derived CO<sub>2</sub> (p = 0.001), and phosphorus and nitrogen limitation both could intensify MAOM mobilization and mineralization by plants. Researchers also explored the interaction of mycorrhizal and BYDV infection and developed an assay for visualizing (via fluorescence) the root-induced release of complex organic molecules from established associations with ferrihydrite. Researchers are currently using the model ecosys to explore the ecosystem-scale implications of altered kinetics of binding and release of OM to and from minerals, and altered capacity for OM binding, for C and nutrient cycling in grasslands and forests. Root-induced mobilization of MAOM has large potential to affect the productivity of ecosystems and the fate of large reserves of C stored in soil.

### Measured and Modeled Responses of Tropical Plant Carbon Balance at the TRACE Site to Long-Term Experimental Warming and Hurricane Disturbance Recovery

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The team is using a unique understory warming experiment along with numerical modeling to determine how tropical forest plants respond to long-term warming and hurricane disturbance in Eastern Puerto Rico. The Tropical Responses to Altered Climate Experiment (TRACE), which uses infrared heaters to warm understory vegetation +4 °C above ambient temperatures, was hit by two major hurricanes in September 2017. Researchers measured plant structure and physiological responses to changing post-hurricane canopy dynamics and experimental warming. They also used the nutrient-enabled Functionally Assembled Terrestrial Ecosystem Simulator (FATES-CNP) to determine how these changes reflect overall carbon exchange and nutrient fluxes in the system. Six years post-hurricane, in situ measurements showed warmed plots were half the height of control. Photosynthesis declined by ~60% in response to closing canopy conditions following the hurricanes and showed a ~30% decline in response to experimental warming. Neither photosynthesis nor plant respiration acclimated significantly to warming or hurricane disturbance; however, root biomass was reduced in warmed plots leading to ~50% reduction in overall ecosystem-level root respiration for warmed plots. Using site-specific data to parameterize the ELM-FATES model, researchers found that +4 °C warming simulations had lower biomass, productivity, and respiration than ambient simulations when there was a hurricane disturbance every 10 years. These changes in biomass, productivity, and respiration, due to warming do not necessarily confer reduced net ecosystem productivity (NEP), which was not different between warmed and ambient simulations. Researchers found that NEP fell from  $\sim 2.5$  g m<sup>-2</sup>d<sup>-1</sup> in base-FATES model runs to near zero in nutrient-enabled model runs (FATES-CNP), driven largely by heterotrophic respiration. This suggests that including more advanced soil processes into the FATES model has large effects on ecosystem processes. Overall, the team found that plant carbon exchange processes acclimated quickly to changes in post-hurricane canopy dynamics, but that warming induced limited physiological acclimation responses.

### Synthesizing Bryophyte Functional Response to Environmental Variation to Improve Terrestrial Carbon Cycle Modeling

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Scientific understanding of current and future drivers of carbon (C) cycling at ecosystem and global scales relies on the ability of Earth system models (ESMs) to accurately represent plant-environment interactions and feedbacks. Bryophytes (mosses and their relatives) significantly affect C cycling, storage, and biogeochemical responses to global change across terrestrial ecosystems, but have remained unrepresented in ESMs. The central aim for this project is to conduct a global synthesis of bryophyte-C cycling processes, their drivers, and their responses to change. The objectives are to (1) leverage existing datasets to generate a database of bryophyte processes that relate to C cycling; and (2) elucidate, analyze, and test key relationships between bryophyte functional processes and environmental variables suitable for inclusion into ESMs and development of a novel bryophyte plant functional type. The preliminary analysis of available literature revealed over 3000 bryophyte functional trait records published since 1980 that are directly (e.g., NPP, biomass, Vcmax, decomposition; 1020 records) or indirectly (e.g., nitrogen content, water holding capacity; 2072 records) related to the C cycling metrics the team intends to develop for bryophyte-specific ESM functions. Researchers located bryophyte-C cycling records present in all focal ecosystems (boreal forest, n=732; Northern latitude, n=630; peatland, n=1232; dryland, n=498) and across all of the bryophyte growth forms (acrocarp, i.e., upright-growing shoots; peat moss; feather moss; biocrust) on which the team will focus for this synthesis.

Preliminary findings suggest bryophytes play relevant roles in terrestrial C cycling and data are available in the literature that characterize key bryophyte processes important to the C cycle across major terrestrial biomes.

#### Predicting Hot Spots and Hot Moments of Biogenic Gas Accumulation and Release in a Subtropical Ecosystem Using Airborne Ground-Penetrating Radar

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Peatlands are major terrestrial carbon (C) stores and large natural producers of biogenic greenhouse gases (e.g., methane; CH<sub>4</sub> and carbon dioxide; CO<sub>2</sub>), which accumulate in the soil matrix and subsequently release to the atmosphere. While several conceptual models have been developed over the last 2 decades, identifying hot spots and hot moments for the accumulation and release of biogenic gases are limited in peatlands, likely due to the lack of effective noninvasive methods available to be deployed at reasonable temporal and spatial scales for such an identification. This project has been testing a small unoccupied aircraft system (sUAS)-based ground-penetrating radar (GPR) prototype for imaging hot spots of gas accumulation in the Everglades, as representative peat soils in subtropical wetland ecosystems. After several delays related to changes in drone legislation in Florida, field campaigns in 2023 provided (1) a seasonal GPR time-lapse dataset collected over a 140 m by 140 m grid in two project sites that show gas content distribution ranging between 2 to 18% during the dry season, shifting to 6 to 28% during the wet season; (2) CH<sub>4</sub> fluxes directly inferred from gas traps ranging between 16 to 80 mg CH<sub>4</sub> m<sup>-2</sup> d<sup>-1</sup> with values almost three times larger in identified hot spots characterized by higher GPR inferred soil gas content; and (3) coincident optical sUAS based multispectral imagery products with five spectral channels (red, green, blue, near infrared, and red edge) and a resolution of 1 foot that will be combined with GPR and field measurements to identify the relationship between the remotely sensed surface reflectance and gas fluxes.

This study also further tested airborne GPR measurements in monoliths under controlled laboratory conditions. Overall GPR gas content distribution in the soil was strikingly similar to field conditions and ranged between 12 to 34% gas content that resulted in gas flux releases up to 82 mg CH<sub>4</sub>  $m^{-2} d^{-1}$  (as directly inferred from gas traps), and higher fluxes once again coinciding with areas of higher GPR inferred gas content. Measurements will be expanded both in the field and laboratory to monitor gas content dynamics in the identified hot spots. Researchers will further analyze (1) gas samples for CH<sub>4</sub> metabolic pathways; and (2) how soil matrix may influence gas distribution via X-ray computed tomography (via a limited scope proposal submitted to the Environmental Molecular Sciences Laboratory).

#### Virtual

#### A Research Agenda for Improving the Representation of Plant Hydrodynamics in Earth System Models

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Plant traits linked to drought tolerance vary widely among different species but also among and even within populations of a single species. This variation is driven partly by antecedent moisture conditions and partly by the pedoclimatic conditions in which the plants grow. While researchers have recently implemented frameworks for simulating plant hydraulics in Earth system models, the frameworks depend on fixed trait values of variable quality, and the data needed to assess and validate these new models are largely lacking. Here, the team discusses how models simulate plant hydraulics, focusing on their strengths, weaknesses, and data needs, and identifies data gaps that limit confidence in their output. Researchers identify field and laboratory research needs related to these models and model evaluation workflows that can build confidence in models' ability to represent plant responses to current and future environmental conditions. To enable more realistic simulation of plant hydraulic responses to water stress in models, the research community should provide model-compatible datasets of key plant hydraulic traits and status for model evaluation, parameterization, and validation. Researchers should use these data to pinpoint ecosystem responses to a changing hydroclimate by addressing both long-term climatic drying and episodic extreme droughts.

# Plant-Mediated Hydraulic Redistribution: A Valve Controlling Watershed Solute Transport?

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Plants passively move water in the subsurface from wet to dry soil via their roots in a process known as hydraulic redistribution (HR). This passive redistribution of soil water may have important implications for a soil's carbon carrying capacity, nutrient exchange, and soil structure, particularly in seasonally water-limited environments such as the Mediterranean climate of the western United States. Soil moisture is an important regulator of microbial activity, organic matter decomposition, biogeochemical cycling, and soil properties. The objective of the project is to elucidate the relationship between HR, soil carbon and nutrient dynamics, and soil properties through a multi-year study with in situ data collected from two adjacent hillslopes at Watershed 10 of H.J. Andrews Experimental Forest in Oregon, USA. Here, recent work has revealed two types of ecohydrological functions associated with high and low HR among the hillslopes. Where trees have access to groundwater, moisture in the upper soil profile vary by nearly 2% between night and day. In contrast, hillslopes where tree access to groundwater is inhibited experience a daily moisture increase in the upper soil of <0.5%. To meet objectives, the team relies on the combination of multidisciplinary monitoring to quantify hydraulically redistributed water and its relationship to soil structure and biogeochemistry.

In summer 2023, the team began monitoring sap flow, soil moisture, CO<sub>2</sub> soil concentration, matrix potential, and soil and tree self-potential. The team also assessed soil structure and chemistry through X-ray computed tomography and high-resolution carbon and nutrient pool characterizations. These measurements are being acquired in four sites, two on each slope with a first site close to the river and a second uphill, where the vegetation have more limited access to groundwater. Last summer's data provide first insights of interactions between trees, soil water, and geochemical dynamics. Additionally, the classification of soil physical and hydrologic properties via field and laboratory analysis has revealed distinct differences between rooting patterns and soil structural properties between high- and low-HR hillslopes. The team finds that high-HR sites tend to have more homogeneous rooting patterns, where low-HR sites have distinct trends in coarse- and fine-root patterns with depth. This result suggests that where water is more limited, roots may have more targeted rooting strategies. Furthermore, in low-HR sites, it appears that more root mass is dedicated to fine, non-woody absorption roots. High-HR sites also tend to have a higher soil clay fraction and smaller overall soil aggregate distribution than low-HR sites. Selfpotential monitoring highlights water flows from the soil to the tree. Initial analyses show that upward water flows are greater at sites near the stream and a strong contrast between high- and low-HR slopes. Combined, these data will help scientists understand how surface vegetation influences subsurface water fluxes with the goal of identifying how these biologically mediated water fluxes may, in turn, alter soil-carbon dynamics and soil physical properties.

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

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Methane (CH<sub>4</sub>) is one of the most important greenhouse gases and more than 30% of its total emissions originate from wetlands. There is high uncertainty in the contribution of mineral soil wetlands to global CH<sub>4</sub> budgets. The project objectives are (1) to improve the understanding of the controls on CH<sub>4</sub> fluxes in forested mineral soil wetlands; and (2) to better understand the effects of landscape position and forest composition on the CH<sub>4</sub> fluxes between terrestrial ecosystems and the atmosphere. Using a coupled modeling-experimental approach, researchers are measuring the spatial and temporal dynamics of CH<sub>4</sub> fluxes in soils and woody structures (stems and knees) of temperate bald cypress (Taxodium distichum) and other bottomland hardwood stands and incorporating measurements into an ecosystem model to improve the model representation and predictions of CH<sub>4</sub> fluxes. Soil collars and custom-built chambers were installed in the stems and knees of trees along four sites that span a hydrologic gradient from the terrace to the stream channel in western Kentucky's Clarks River National Wildlife Refuge (CRNWR). The team found significant differences in soil  $CH_4$  fluxes (p-value < 0.02) between the bald cypress stand and the other species stands (p-value < 0.02), but no significant differences in stem  $CH_4$ fluxes among species (p-value = 0.25) during the drought year. These results showed a higher average soil CH<sub>4</sub> uptake rate in high knee density areas compared to no knee areas (p = 0.004) that can offset the observed knee CH<sub>4</sub> emission. Researchers found no statistically significant difference between soil fluxes during drought and after historic flooding events (except for the post oak site), but the flooding event can enhance stem and knee CH<sub>4</sub> emissions. The team will use ongoing monitoring to improve understanding of soil-vegetation interaction in hardwood bottomland wetlands and incorporate these functions into ongoing processes-based modeling efforts.

#### Rhizosphere Carbon Fluxes Under Drought and Hydraulic Redistribution Conditions

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Hydraulic redistribution (HR) is the passive movement of water from wet soil regions to dry soil regions (for example from deep soils at the water table to dry surface soils) using plant roots as conduits. It is well appreciated that HR plays an important role in plant growth and survival during periods of drought but less is known about how HR sustains microbial life in the soil. HR provides water to microbes in the rhizosphere, and it also may flush root exudates into the rhizosphere. The central hypotheses behind this research are (1) plants produce higher quantities of root exudates when undergoing HR; (2) the flow of water during HR carries these exudates farther than they would normally diffuse into the soil, expanding the rhizosphere, and; (3) HR-delivered exudates and water sustain microbial activity during drought with important implications for carbon cycling in soils. The experimental work on this project has focused on developing and refining analytical methods for the analysis of root exudates under both HR and non-HR conditions and preparing specimens in the greenhouse for performing these experiments. Working with collaborators at Environmental Molecular Sciences Laboratory (EMSL), researchers have developed novel exudate collection and FT-ICR-MSI analysis methods that permit imaging of root exudation along the root network. Researchers have also developed an extensive LC-MS based metabolite library and analytical workflow for processing of exudate samples.

The modelling work on this project has coupled the Carbon, Organisms, Rhizosphere, and Protection in the Soil Environment (CORPSE) soil biogeochemical model to a 1-D advection-dispersion model to model exudate transport and transformations in the rhizosphere. This has been coupled in turn to the TREES ecohydrological model. This model has been tested against data from several FluxNet sites and will be used to model root-rhizosphere processes under the greenhouse conditions of the experiment.

#### Virtual

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

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Rapid warming of high-latitude regions is increasing plant trait variation across local to regional scales. Due to the critical role plant traits (e.g., leaf nitrogen, specific leaf area) have in gross primary production and plant and soil respiration, understanding the spatial patterns of trait variability across changing tundra ecosystems is essential for improving the performance of Earth system models. This project aims to improve the representation of trait variation in models by characterizing directly observable plant traits from remotely sensed data and predicting unobservable (e.g., belowground) traits. This trait information will be integrated into the Terrestrial Ecosystem Model to quantify and predict regional carbon balance in the Alaskan tundra.

In 2021 and 2022, the team established eight sites representing dominant plant community types in northern Alaska. Five of the sites have been sampled; the remaining sites will be sampled in 2024. At each site, researchers measured species percent cover, canopy height, and soil microenvironmental parameters and collected leaf and root samples to characterize traits at the species, functional type, and community levels. Each site was also imaged using hyperspectral and light detection and ranging sensors onboard an uncrewed aerial system (UAS).

UAS-derived plant trait maps represent well ground-based observations of leaf traits and aboveground biomass (root traits are currently being measured), explaining 43 to 87% of the trait variability across sites. To upscale plant traits, the team merged site-specific trait maps and models with Airborne Visible Infrared Imaging Spectrometer-Next Generation (AVIRIS-NG) data.

Preliminary results suggest the accuracy of plant trait retrieval via remote sensing will be trait-specific and vary by ecoregion. This highlights the necessity of incorporating local-scale plant trait variability for accurately modeling regional-scale plant trait variation. This research will improve the ability to map plant trait variation across vast regions of the Arctic, furthering understanding of highlatitude carbon-climate feedbacks.

## Improving Environmental System Science Approaches to Evapotranspiration Partitioning Through Data Fusion

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This project aims to address the uncertainty in estimates of T/ET, which is the ratio of transpiration (T) to evapotranspiration (ET) flux in hydrologic models. Previous research has shown that models often exhibit compensating errors such that total ET estimates have relatively small biases in comparison to eddy covariance tower ET measurements, yet exhibit strongly divergent T/ET ratios. This uncertainty in T/ET ratios limits the utility of Earth System Models in applications that heavily rely on this partitioning, including investigations of soil moisture dynamics, vegetation dynamics and productivity, food security, and watershed hydrologic response, among others. To provide new insight for mechanistic modeling of ET partitioning within Earth System Models and improve future predictions, this project will evaluate different T/ET partitioning methods through cross-site synthesis. Researchers use these to produce benchmark T/ET data products at long-term research sites and in an upscaled estimate, global T/ET estimates derived from calibrated E3SM Land Model (ELM) simulations under current and future conditions. In doing so, the project will provide fundamental advancements in the characterization of process-based model uncertainty, improvement

of modeling with T/ET fusion estimates, and estimation of future declines in T/ET under changing climates. The proposed research will leverage data from AmeriFlux networks and other networks and aligns with the DOE Model-Experiment (ModEx) paradigm. The project addresses ESS Science Research Area 3: "Synthesis Research for Transferable Insights" and will improve understanding broadly across the water, carbon, and energy cycles.

#### Are Trees Dormant During the Dormant Season? Determining the Importance of Plant Nutrient Uptake in Changing Cold Seasons in Cold-Region Catchments

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Most Earth system models tie plant nutrient uptake to photosynthetic demand and predict that uptake ceases over winter. However, plants may be more active belowground during winter than previously recognized. Yet, the extent of plant nitrogen (N) uptake during the dormant season is not known, nor how it varies with plant traits or in response to warming winters. Researchers are conducting a set of experiments and modeling activities to characterize cold-season plant N uptake, its controls, and its response to shrinking snowpacks in seasonally cold temperate forests. The team's overarching hypothesis is that temperate trees take up biogeochemically important amounts of N over winter and that this uptake changes along with winter climate conditions. Researchers are testing this hypothesis with <sup>15</sup>N tracer studies of cold-season N uptake, snowpack manipulation experiments, and the equilibrium chemical approximation (ECA) version of the E3SM land model. First (Objective I), researchers are both simulating (ELM-ECA) and measuring (<sup>15</sup>N tracers) winter plant N uptake by juvenile and adult trees spanning a range of plant functional traits. Next, at the ecosystem scale (Objective II), researchers are both simulating (ELM-ECA) and measuring (<sup>15</sup>N tracers) competition for N among mature trees, microbes, and gaseous and hydrologic N losses in response to experimentally reduced winter snowpacks at Arnot Forest, NY, and Hubbard Brook, NH, two watersheds with contrasting stream nitrate seasonality. Last (Objective III), the team will use ELM-ECA to assess how cold-season plant N uptake and changing winter snowpacks will alter terrestrial carbon and nitrogen dynamics under future scenarios of additional warming and rising atmospheric CO<sub>2</sub>. Together, the proposed activities will test and strengthen E3SM-ELM representation of plant N uptake, which is one of the largest annual N fluxes in

terrestrial ecosystems and a central constraint on terrestrialcarbon sequestration.

#### Understanding the Geochemical Basis for Soil Organic Matter Storage at the Global Scale

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Terrestrial ecosystems capture atmospheric CO<sub>2</sub> and incorporate it into soil organic matter (SOM). SOM can be decomposed by microbes—returning carbon (C) to the atmosphere—or stabilized by minerals and retained in soil. Predicting the balance between decomposition and SOM retention in soil is critical to forecasting future atmospheric CO<sub>2</sub> levels yet remains a major challenge for biogeochemical models. These models use climate and soil clay content to constrain rates of SOM cycling; however, it is the overall reactivity of soil minerals and not simply clay content that controls SOM retention. Incorporating the effects of mineral reactivity on SOM cycling at the global scale is not currently possible because of a lack of detailed global maps of the soil geochemical environment. To close this knowledge gap, researchers have synthesized seven geochemical datasets that cover five continents. With this combined database (n=21,000+ observations), researchers will test the extent to which geologic factors influence soil mineralogy and SOM storage. Specifically, the team will use this harmonized geochemical database to model and predict soil mineralogy and mineral reactivity globally. These modeling efforts will rely on a process-based geochemical model complemented by machine-learning derived predictions. The team will use the model outputs to evaluate how patterns and trends in mineral reactivity relate to SOM storage. Researchers will develop a publicly available version of the final harmonized database and derived model predictions to be hosted by the Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE). The results will provide insight into the geologic and topographic controls on C dynamics important for climate predictions.

Furthermore, soil mineralogy data products will make models better equipped to include geochemical data and analysis of SOM stabilization.

# Linking Field Experiments and Modeling to Understand the Role of Hydraulic Redistribution in Temperate Forests

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Plant-mediated hydraulic redistribution (HR) may play a significant role in maintaining photosynthesis and transpiration rates during periods of drought. Climate projections suggest that warmer conditions will consistently increase water stress during the growing season, which may exacerbate droughts and increase the importance of HR in buffering periods of water limitation. However, these processes are currently not well constrained in Earth system models which could be a source of the well-known uncertainty in simulations of soil moisture states and of water and carbon fluxes.

Researchers use field experiments to better understand the prevalence and magnitude of HR across tree species, tree sizes, and drought durations in three temperate forest species (*Juglans nigra, Quercus rubra* and *Acer saccharum*), representing contrasting hydraulic strategies, by measuring soil and plant hydrologic and hydraulic properties and fluxes. Trees are instrumented with sap flow probes at three locations ranging from the roots to the lowest branch, psychrometers and water content probes. To facilitate the soil moisture gradient that is necessary for HR to take place, 50% of the trees are equipped with plastic skirts that prevent water from replenishing upper soil layers.

Simultaneously, researchers use model sensitivity experiments to explore the hypothesized water resource competition between nighttime stomatal conductance, recharge of plant-water storage and hydraulic redistribution. Better understanding of this partitioning and its influence on fluxes is a key first step to improving model parameterizations of HR. Researchers use two models that couple with the E3SM land model (ELM); the parameter-rich FATES-HYDRO hydrodynamics model and ELM with a new, simpler, plant hydraulic stress (PHS) representation. Researchers provide an overview of the field and model experimental designs and of the results and lessons learned available at this early point in the project.

#### Investigating Cross-Scale Dynamics at Terrestrial-Aquatic Interfaces in Temperate Forests

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Terrestrial-aquatic interfaces are critical sites of biogeochemical processing, and the location of these interfaces is increasingly impacted by rising total annual precipitation and extreme rain events that rapidly move the water table. Small and ephemeral wetlands are particularly dynamic in space and time within temperate forests. In the saturated zone below the water table, conditions are anaerobic, and methane (CH<sub>4</sub>) is produced. Dissolved gas may diffuse or bubble up to the water table or escape to the atmosphere through plant roots and stems. In the unsaturated zone above the water table, conditions are oxic, carbon dioxide (CO<sub>2</sub>) is produced, and CH<sub>4</sub> is oxidized. Additionally, CH<sub>4</sub> transported by ebullition and tree stems have high variation across the landscape and through time, and the mechanisms driving plant-mediated methane transport are not well understood.

In this project, which began in September 2023, researchers are conducting cross-scale field measurements of methane dynamics at the Harvard Forest in Petersham, MA within uplands, ephemeral wetlands, and two small perennial wetlands: an approximately 14-thousand-year-old forested peatland and an approximately 20-year-old beaver-constructed wetland. Researchers are leveraging data and infrastructure from core AmeriFlux towers to add new ecosystem-scale measurements of  $CH_4$  and  $CO_2$  exchange and are measuring the lateral flow of carbon (C) in gaged streams and  $CH_4$  flux from tree stems. At the process-scale, researchers will characterize rates of  $CH_4$  production, consumption, ebullition, and diffusion and will develop a novel reactive transport model to represent these processes.

Future work will synthesize new field measurements within a spatiotemporal modeling framework that brings together process-based measurements with net  $CH_4$  flux constraints from eddy flux towers and lateral flow data. The observational design will facilitate understanding of the dynamics of  $CH_4$  within this complex ecosystem that dynamically changes across space and through time with precipitation.

#### Ectomycorrhizal Production Phenology Follows Roots but Varies by Host Tree Species

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Mycorrhizal symbioses account for 15 to 45% of forest productivity, but empirical estimates remain uncertain. Belowground phenology, which differs notably in timing from leaf production, constrains the temporal distribution of carbon allocation to roots and fungi. Mycorrhizal root and hyphal production can also differ by plant functional type, tree and fungal species, and environmental conditions. To improve the collective ability to model land carbon dynamics, researchers are measuring mycorrhizal fungal phenology with monthly sampling of roots and soils across a diverse set of 10 monodominant stands of common temperate tree species at the Morton Arboretum in Chicago, IL. Annual sampling dates align with key tree phenophases and span a broad range of typical soil moisture and temperature values for temperate forests, including a drought period followed by a pulse rain event. The team estimates hyphal production via minirhizotron image scans and qPCR and identify mycorrhizal fungal community shifts with high-throughput amplicon sequencing.

Overall, mycorrhizal root and hyphal production is seasonal, and appears to vary more strongly by tree species than by plant functional type. Net hyphal production peaks in midfall, after soils begin to rewet following mid-summer dry down. Ectomycorrhizal hyphae and rhizomorphs peak in production either after or in synchrony with peak fine root production, depending on the specific host tree species. In some cases, a peak in rhizomorph production in spring with little hyphal growth was observed. Researchers expect peak hyphal diversity and production in fall, and for this to be dominated by a few ectomycorrhizal fungal genera, including *Lactarius, Suillus*, or *Amanita* as in some previous studies. Future work will link below- and aboveground tree phenology as well as identify drivers of intra- and inter-annual compositional shifts in mycorrhizal fungal communities.

#### Unraveling the Mechanisms of Below- and Aboveground Liana-Tree Competition in Tropical Forests

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Trees and lianas dominate the canopy of tropical forests and comprise the majority of tropical aboveground carbon (C) storage. These growth forms respond differently to variation in climate and resource availability. The overarching objectives of this project are (1) to carry out an observational campaign to advance the understanding of liana traits and strategies; (2) develop a liana-enabled forest dynamics model that leverages the observations; and (3) to engage with the Earth System Modeling (ESM) community to plan for the eventual inclusion of lianas into ESMs. Here, researchers report on five activities which have brought the team closer to meeting these objectives:

- (1) The team measured and analyzed liana traits. Researchers found marked differences between lianas and trees in terms of their hydraulic traits and xylem anatomical traits. The team also identified significant variation in hydraulic traits across liana species.
- (2) Researchers incorporated these results into a reduced 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) The team measured tree growth and liana colonization status of over 1,700 trees at a study site in Guanacaste, Costa Rica. It was 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) Researchers incorporated lianas into the TROLL forest dynamics model. TROLL represents the threedimensional canopies of trees and lianas. Researchers have carried out a sensitivity analysis and tested the model's ability to simulate observed patterns.
- (5) The team simulated liana-enabled forest dynamics in TROLL. These dynamics included the ability of lianas to colonize multiple trees and the ability of trees to shed lianas.

# Improving Models of Stand and Watershed Carbon and Water Fluxes with More Accurate Representations of Soil-Plant-Water Dynamics in Southern Pine Ecosystems

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Despite strong fundamental knowledge about the key processes through which plant hydraulics affect water uptake and productivity, researchers currently lack several key components necessary for a predictive understanding of ecosystem response to future climate conditions. These components include mechanistic understanding of plant-mediated hydraulic processes in under-studied systems and representations of biophysical factors affecting coupled water-carbon cycles in models. This project focuses on longleaf pine ecosystems, once a dominant forest type in the southeast U.S. that is undergoing large-scale efforts to be restored through much of its native range. During project year two, the team accomplished several goals with a focus on field measurements. Researchers installed an extensive array of tree root and trunk sap flow sensors, including some capable of detecting bidirectional root flow at night. The team also installed moisture probes in tree trunks and soil profiles to quantify tree and soil water storage. A soil respiration and evaporation experiment was initiated to collect pretreatment data; next year the roots will be severed to eliminate root flow in the treatment plot. These measurements will determine whether hydraulic redistribution (HR) affects shallow soil moisture and subsequently respiration or evaporation. Researchers also successfully quantified tree canopy leaf photosynthetic parameters by harvesting canopy branches and measured predawn and midday leaf water potentials, which are needed for modeling HR. Root mass and area profiles were measured in three replicates up to one meter. Soils were sent to the University of Indiana to measure hydraulic parameters. Data collection at AmeriFlux towers US-HB2 (mature longleaf) and US- HB3 (young longleaf) continued uninterrupted. The team installed a new understory eddy covariance system at US-HB2 with a new PhenoCam to track phenology of the longleaf understory.

Measurements resumed at AmeriFlux tower US-Akn at Savannah River National Laboratory, and a soil moisture profiler was installed. Advances in model development include an ecosystem respiration module accounting for both autotrophic and heterotrophic respiration, as well as a stochastic precipitation module described by the Marked Poisson process that will translate the precipitation results from Energy Exascale Earth System Model (E3SM) climate simulations to evaluate the impacts of future climate scenarios on the ecosystem water and carbon fluxes.

## Integrating Process-Based and Machine Learning Approaches for Estimating the Global Methane Soil Sink

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Methane (CH<sub>4</sub>) voxidation by microbes is the second largest sink in the global CH<sub>4</sub> budget, but the magnitude and variability in soil CH<sub>4</sub> oxidation are uncertain. Recent studies identified an overlooked CH<sub>4</sub> soil sink in diverse terrestrial ecosystems, attributed to high-affinity methanotrophs growing on atmospheric CH<sub>4</sub> in dry mineral soils. The current estimation of the global methane soil sink is ~30 Tg yr<sup>-1</sup> but with considerable uncertainty (7 to >100 Tg yr<sup>-1</sup>) from previous studies. Accurately quantifying the soil sink is vital to reduce the bias in current and future global CH<sub>4</sub> budgets.

Process-based modeling and machine learning approaches have been widely used to quantify methane fluxes on regional and global scales, but both approaches show their limitations. Specifically, results show large uncertainties in process-based estimation due to parameter optimization and governing microbial processes. Results further show limitations of the machine learning approach due to out-ofsample prediction failure and low interpretability with key responses that govern soil CH<sub>4</sub> oxidation processes.

In this context, the emerging field of Knowledge-Guided Machine Learning (KGML) offers a promising hybrid modeling method, integrating the strengths of process-based models, machine learning techniques, and multisource datasets. In this presentation, researchers introduce novel KGML framework, designed to incorporate biogeochemical knowledge into machine learning algorithms effectively. The framework integrates direct measurements from the FLUXNET-CH<sub>4</sub> and chamber datasets, along with indirect measurements of global soil temperature and moisture, to train and validate the model. Through this innovative approach, researchers aim to enhance understanding of soil methane oxidation processes, reduce uncertainties in methane budgets, and foster more accurate projections of global CH<sub>4</sub> dynamics.

#### Virtual

#### Context-Aware Deep Learning Framework for Earth System Model Data Compression and Downscaling

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To conduct risk assessments and design adaptation plans against changes in climate patterns and their impacts on society, future local and regional projections of climate change hold great importance. Earth system models (ESMs) that currently run on massive supercomputers are used to generate both global and regional projections at different horizontal and vertical resolutions. These models simulate Earth's past climate and project future scenarios, considering changes and uncertainty in atmospheric greenhouse gas emissions. ESMs are computationally expensive and require significant data resources [e.g., 1 month of simulation data using DOE's Energy Exascale Earth System Model (E3SM) equals 14 gigabyte storage space plus memory-intensive visualization] even when operating at lower horizontal resolution (LR). For these reasons, data compression and dynamical and statistical data downscaling have been extensively practiced. In this work, the team proposes a novel two-stage framework based on deep learning to overcome this dual challenge. This framework combines an implicit neural representation (INR) and a super-resolution generative adversarial network (SRGAN). In stage 1, INR is used to compress the E3SM data by saving the weights derived from a neural network, which is trained to excessively conform to the data while maximizing overfitting. In the next stage, SRGAN is used to downscale the LR data (obtained by inferring INR) into a higher horizontal resolution (HR) to generate a more accurate representation of the ESM data for regional investigations. The primary objective of this work is to evaluate the performance of this two-stage framework in compressing and downscaling ESM data with a specific focus on surface temperature profiles derived from E3SM. Results show that the proposed framework can achieve compression gain up to four orders of magnitude with a considerable peak-to-signal ratio and generate HR profiles using the LR counterparts with significant accuracy measured based on the Learned Perceptual Image Patch Similarity metric.

#### Empirical Measurements and Model Representation of Hydraulic Redistribution as a Control on Function of Semiarid Woody Ecosystems

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Earth System Model (ESM) projections of ecosystem responses to climate change require knowledge of biomes that vary in climate sensitivity. Drylands influence the trend and interannual variability in global sink strength but are difficult to represent in ESMs. Incorporation of plant-mediated hydraulic redistribution (HR; flow in plant roots from wetter to drier soil) can improve ESM performance in drylands. Researchers combine measurements of sap flow, soil moisture, and ecosystem-scale net ecosystem exchange (NEE), gross primary production (GPP), and ecosystem respiration *Re*, and use data assimilation to develop the Terrestrial Ecosystem (TECO) model to address three objectives:

- Understand the controls on HR in species and biomes across a range of semi-arid western woodlands/forests. At four AmeriFlux sites, supplemental depth profiles of volumetric soil moisture and soil water potential sensors, colocated with measurements of root sap flux capture patterns of HR, the physical factors driving it, and related ecosystem function as HR varies.
- (2) Quantify seasonal patterns of HR across dryland species and biomes to determine when HR affects soil moisture dynamics and ecosystem function. Researchers measure HR from lower elevation juniper savanna and pinon-juniper woodlands to higher elevation ponderosa pine and mixed conifer forests, leveraging data collection at tower sites and supplementing these efforts with additional soil and sap flux measurements.
- (3) Scale plant-level patterns in HR to ecosystem-level NEE, GPP and Re in response to precipitation anomalies. Incorporating HR into TECO predicted upward HR with increased shallow soil moisture during dry periods and a corresponding reduction in deep soil moisture. After rainfall, the TECO+HR model predicted downward HR. Introducing HR also predicted noticeable effects on carbon fluxes alleviating the impact of drought, resulting in a predicted 8 to 21% increase in GPP and NPP, and a 5 to 12% rise in Re. These findings highlight the significant role of HR in influencing both soil moisture dynamics and carbon fluxes in an ecosystem.

# Impaired Water Relations in Carbon-Limited Ponderosa Pines: Implications for Belowground Interactions

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How drought kills trees is not fully understood. Drought reduces carbon (C) assimilation, but C demand for energy continues, and plants eventually use their stored nonstructural carbohydrate (NSC) reserves to meet demand. Whether depletion of stored NSC impairs turgor maintenance in the field is not known, but it is critical for models to predict vegetation responses to drought. Researchers tested whether depletion of stored NSC impairs water relations in ponderosa pine in the field, and whether common mycorrhizal networks (CMN) could mediate these effects on surviving trees when connected trees die and cease to supply C below ground.

In the summer of 2022, researchers subjected trees under ambient precipitation and experimental drought to either full sun or to 8 weeks of shade. The team measured NSC content in needles, pre-dawn needle water potential, osmotic potential, and turgor pressure prior to shading and at weekly intervals for 8 weeks. In the summer of 2023, researchers girdled trees under ambient precipitation and under drought, and tested whether connected neighbor trees became NSC depleted and the consequences on drought tolerance.

In 2022, shade depleted stored NSC in ambient trees but not under drought. NSC depletion impaired osmoregulation capacity in shaded trees but not in nonshaded trees, suggesting that negative effects of NSC depletion on drought tolerance occur only when trees are C limited. In 2023, girdling reduced C supply underground, and tentative results indicate that neighbor trees connected through CMN became NSC depleted, and their turgor maintenance was compromised. Researchers demonstrate that stored NSC depletion can impair water relations in ponderosa pine in the field, and tentatively suggest that when some trees die, CMN could mediate C limitation and impair drought tolerance in connected surviving neighbors.

# Mycorrhizal Phenology Under Altered Snowmelt Timing

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The warmer and drier conditions created by climate change shift plant phenologies through altered environmental cues, potentially creating novel organismal interactions between plants and mycorrhizal fungal partners. The symbiosis between plants and arbuscular mycorrhizal (AM) fungi is fundamental for plant access to labile nutrients. During the early spring in alpine ecosystems, snowmelt creates a flush of soil resources (water, nitrogen, and phosphorus), which AM fungi provide to the plant host in exchange for photosynthate carbon (C). This snowmelt date is advancing as the climate warms, which researchers hypothesized would result in asynchrony of plant-mycorrhizal fungal nutrient cycling. The team advanced the snowmelt date by 10 days in a Colorado subalpine meadow using shade cloth. Throughout the following growing period (May to September), the team tracked new root and hyphal growth with ingrowth cores and composition of the soil microbiome with amplicon sequencing (loci: ITS - general fungi, SSU - AMF). Researchers coupled this to simultaneous measures of mineral and microbial biomass nitrogen. Shotgun metagenomic sequencing was also used to track the genetic inventory of microbial biogeochemical functions, revealing significant temporal variation of bacterial nitrogen cycling genes. The team found that the standing stock of AM hyphae was highest under snowpack in early May, steadily decreasing throughout the growing period. Snowmelt treatment did not impact this metric of AM growth but did decrease hyphal density of saprotrophic fungi during the senescence period in mid-September. The team will detail how altered snowmelt impacted the synchrony of root and fungal growth and the resulting impact on AM community composition, soil nitrogen availability, and microbial nitrogen cycling.

#### Student

### Assessing Rangeland Function under Altered Precipitation Regimes: Can a Deluge Rescue Forage Production Following Catastrophic Loss of the Dominant Species?

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The frequency of co-occurring droughts and deluges (i.e., large rainfall events) are projected to increase due to atmospheric warming. The potential ecosystem-scale impacts of these compound extremes are largely unquantified, yet they could be largely responsible for intra- and interannual variation in biogeochemical cycling. Ecosystem functionality is particularly vulnerable to altered precipitation regimes in water-limited systems such as the semi-arid shortgrass steppe of the western Great Plains. Key determinants of ecosystem stability are dominant species which, by definition, play a vital role in driving functionality (e.g., carbon storage via biomass production). Evidence has shown that climatic extremes can push dominant species to their physiological limits, leading to their loss from the system. This project seeks to understand how semi-arid grasslands will respond to compound drought-deluge in the presence and absence of the dominant species.

The proposed study will be initialized in the shortgrass steppe of northeastern Colorado by installing rainout shelters and simulating compound drought-deluge via water addition. Emphasis will be placed on the role of the dominant grass species, Bouteloua gracilis and Bouteloua dactyloides, in driving responses by superimposing a removal treatment that mimics the realistic loss of dominants. Researchers anticipate the addition of a late-growing season deluge to stimulate plant growth, microbial activity, and nutrient cycling, but they do not expect it to fully compensate for the loss of dominants. Aboveground (e.g., productivity and plant community composition) and belowground (e.g., microbial community structure and soil moisture) variables will be measured throughout the study. Investigating multiple trophic levels may lend insight to potential asynchronous responses to climate extremes.

#### Simulating Greenhouse Gas Fluxes from a Terrestrial-Aquatic Interface using Microsite Probability Density Functions and Redox-Reaction Networks

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https://ess.science.energy.gov/summary-of-environmental-system-science- projects-awarded-in-summer-2021/

Terrestrial-aquatic interfaces (TAIs) represent biogeochemically active and diverse systems. Soil microsites regulate oxidation-reduction (redox)-driven biogeochemical transformations and greenhouse gas (GHG) fluxes in TAIs by creating spatial heterogeneity and variations in reaction kinetics. Researchers demonstrate how microsite-scale processes manifest into ecosystem-scale functions and ultimately control GHG fluxes in these dynamic interfaces. The team quantified redox heterogeneity using intact soil cores collected from a TAI near Old Woman Creek, OH and O<sub>2</sub> optodes. Flooding and draining events significantly shifted O<sub>2</sub> distribution, which allowed the team to develop O<sub>2</sub> probability distribution functions (PDFs). By constraining microsite O<sub>2</sub> PDFs in the Dual Arrhenius and Michaelis-Menten-Greenhouse Gas (DAMM-GHG) model, researchers are quantifying spatial (across sites) and temporal (hydrology treatment) heterogeneity of GHG production and consumption processes, and evaluating model performance against observed GHG fluxes in the laboratory. Using microsite O<sub>2</sub> PDFs, the team will explain hot spots and hot moments of GHG fluxes under fluctuating hydrology. Further, researchers are constraining redox reaction network in AquaMEND using soil structural (or pore network) heterogeneity (via X-ray Computed Tomography), and information on alternative terminal electron acceptors (via porewater measurements), and redox potential (via Eh probes). The team will further validate model performance against field measurements of GHG fluxes across the hydrology gradient in Old Woman Creek. The Model-Experiment (ModEx) framework evaluates whether explicitly representing soil microsite PDFs and redox reaction networks improve predictions of GHG fluxes from TAIs.

# Modeling Temperature Sensitivity of Soil Respiration from Two Field-Warming Experiments in Tropics

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Soil respiration is the second largest terrestrial carbon (C) flux. Understanding responses of soil respiration to warming is crucial for evaluating carbon-climate feedback. Warming response of soil respiration is typically modeled using a Q10 function. Generally, observations of the apparent Q<sub>10</sub> of soil respiration are higher for cool vs. warm-climate ecosystems, reflecting expected biophysical controls of Arrhenius kinetics. However, results from two tropical field warming experiments contradict this expectation, both observing extraordinarily high soil respiration responses to in situ warming. Researchers systematically represent the potentially confounding effects of temperature sensitivity of enzymatic reactions, changes in the microbial enzymatic capacity, and substrate supply as they affect microbial decomposition of soil C in tropical forests under warming. Researchers are optimizing the Dual Arrhenius Michaelis-Menten (DAMM) model using data generated from the Soil Warming Experiment in lowland tropical forests in Panama and Tropical Responses to Altered Climate Experiment in Puerto Rico. By including simple representations of measured warming-induced changes in microbial biomass, which affects enzymatic capacity, and soil moisture, which affects substrate diffusion, researchers show that the observed increased soil respiration with warming does not necessarily reflect a change in activation energy  $(E_a)$ , but rather can primarily be the consequence of increased microbial enzymatic capacity. In contrast, optimization of the model without representation of changing microbial biomass would require a higher E<sub>a</sub> in the warmed plots, which is unlikely. The parsimonious modular approach allows researchers to attribute agreement or disagreement of model outputs with observations and specific model functions, as well as identify model structures necessary for skillfully representing temperature-sensitive processes from individual plots to Earth system scales.

# Droughts and Deluges in Semiarid Grassland Ecosystems: Implications of Co-Occurring Extremes for Carbon Cycling

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The overall goal of the research project is to assess how co-occurring drought and deluge climate extremes will impact key carbon (C) cycling processes known to be important for C-climate feedbacks. The team will address this goal via research in the 280,000 km<sup>2</sup> semiarid shortgrass steppe ecoregion located at the western edge of the U.S. Great Plains. Semiarid regions, such as this one, respond strongly to precipitation extremes and play a dominant role in interannual variability of the global land CO<sup>2</sup> sink. The key hypothesis researchers are testing is 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 nitrogen 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, researchers have established 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 year experiment. To scale up from the plot level experiment to the shortgrass steppe ecoregion, researchers are using historical climate data to quantify the regional frequency of potential drought-deluge interactions and remote sensing products (NDVI and Solar Induced Fluorescence) 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, researchers will simulate extreme drought, deluge and drought-deluge perturbations with DOE's E3SM Land Model (ELM). Researchers 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 the 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.

# Eddy Covariance of Methane in Upland and Seasonally Flooded Forests in the Amazon Basin, Working Towards the Contribution of Tree Stems on Ecosystem Methane Fluxes

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Late addition, see full abstract, p. 109

#### Student

#### The Effect of Accelerated Snowmelt on Carbon Cycling Across a Growing Season

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Climate change impacts snowmelt timing, which has cascading effects on ecosystems. Earlier snowmelt can lengthen the growing season of plants or shift plant phenology to earlier in the year but maintain the same season length. The team explored how an accelerated snowmelt date of approximately two weeks impacted the ecosystem respiration, production, and plant biomass in a montane meadow ecosystem over the growing season. Researchers measured NEE (net ecosystem exchange), GPP (gross primary productivity), ER (ecosystem respiration), shrub biomass, graminoid biomass, forb biomass, air temperature, and soil moisture biweekly in five early snowmelt and five control plots from early June to mid-August 2023. The team found that an earlier snowmelt date impacts the productivity of plants by shifting the growing season earlier in the year. However, early snowmelt does not affect overall net ecosystem exchange, as ecosystem respiration remains unchanged.

Using a Bayesian model, researchers found that with earlier snowmelt, gross primary productivity is limited by soil moisture more than in control plots, and the negative effect of drought increases as the growing season progresses. Surprisingly, it was found that an earlier snowmelt date did not significantly affect the plant biomass of any functional group (all long-lived perennials). However, the impact of an earlier snowmelt date on the relative abundance of each plant species could explain the shift in plant productivity. As winters become warmer and snowmelt advances, plant productivity will shift to earlier in the growing season and be limited by decreased soil moisture. Consequences of altered plant phenology on other ecosystem components, including associations with belowground mutualists and nutrient retention in soils, are the targets for the remainder of this grant. This data will allow the team to model the relative importance of abiotic conditions, aboveground, and belowground biota on carbon cycling throughout the growing season in response to accelerated snowmelt.

#### Virtual

# Effects of Fire and Fire-Induced Changes in Soil Properties on Post-Burn Soil Respiration

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https://whitmanlab.soils.wisc.edu/research

Boreal forests cover vast areas of the northern hemisphere and store large amounts of carbon (C). Wildfires affect soil C via combustion and transformation of organic matter during fire and via changes in plant growth and microbial activity postfire. Wildfire regimes in many boreal forests of North America are shifting towards more frequent and severe fires. As wildfire regimes shift, there is a need to link fire-induced changes in soil properties to changes in microbial functions such as respiration to better predict the impact of future fires on C cycling.

The team used laboratory burn simulations characteristic of boreal crown fires on both organic-rich and sandy soil cores collected from Wood Buffalo National Park in Alberta, Canada, to measure the effects of burning on soil properties including pH, total C, and total nitrogen (N). Researchers used 70-day soil incubations and two-pool exponential decay models to characterize the impacts of burning on soil properties and respiration. Laboratory burns successfully captured a range of soil temperatures that were realistic for natural wildfire events. Burning increased pH and caused small decreases in the C to N ratio in organic soil.

Overall, respiration per gram total (post-burn) C in burned soil cores was 16% lower than in corresponding unburned control cores, indicating that soil C lost during a burn may be partially offset by burn-induced decreases in respiration rates. Simultaneously, burning altered remaining C cycles, increasing the proportion of C represented in the modeled slow-cycling versus fast-cycling C pool as well as increasing fast-cycling C decomposition rates. Together, these findings imply that C storage in boreal forests following wildfires will be driven by the combination of C losses during the burn itself as well as burn-induced changes to the soil C pool that modulate postfire respiration rates. The team will also discuss next directions for this project.

# Monitor And Constrain Tropical Ecosystem Sensitivity to Moisture: Progress in Characterizing Ecohydrology of a Tropical Moist Forest Under Experimental Throughfall Exclusion

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How tropical vegetation respond to moisture changes and how these responses in turn regulate ecosystem water dynamics constitutes a major uncertainty in ecohydrological predictions in Earth System Models (ESMs). In this project, the team aims to improve mechanistic understanding of plant-mediated ecohydrology by monitoring and modeling ecosystem dynamics at a new manipulative throughfall exclusion (TFE) experiment at Luquillo LTER station, Puerto Rico. Researchers focus on investigating (1) the coupling between soil moisture and vegetation water content; (2) the relatively unconstrained plant ecohydrological processes such as leaf angle responses to water stress and root hydraulic redistribution; and (3) the implications of site-level manipulative experiment results on modeling longterm vegetation dynamics in the tropics. Field campaigns in 2023 have installed in situ sensors and collected critical pre-treatment data. Researchers now have several months of continuous data from GNSS sensor pairs that can provide one of the first ground-based vegetation optical depth measurements for tropical forests. Researchers have also installed soil moisture and soil water potential sensors that can sample horizontal and vertical heterogeneity in soil water conditions. These point soil moisture measurements agree qualitatively with soil moisture estimates with ground-penetration radar (GPR) from the campaigns, implying the potential of using GPR in monitoring 2D and 3D moisture patterns and dynamics in the system. Additionally, researchers have preliminary stem and root sap flow data from representative species to infer plant hydrodynamics and root hydraulic redistribution, and preliminary terrestrial laser scanning (TLS) suggests it is possible to monitor canopy leaf angle changes under water stress (Yang et al. 2023). These field data and other tropical data such as tree rings provided by additional collaborators (Xu et al. 2024) will be assimilated into ED2.2-hydro and E3SM Land Model-FATES to explore implications of tropical ecosystem sensitivity to moisture constrained by the TFE experiment.

Yang, X., et al. "Leaf Angle as a Leaf and Canopy Trait: Rejuvenating its Role in Ecology with New Technology," *Ecology Letters.* 

# Terrestrial Ecology National Laboratory Projects

# Next-Generation Ecosystem Experiments Arctic

### NGEE Arctic: Integrating Boots-on-the-Ground Observations with the Virtual World of Models to Answer Big Science Questions Across the Arctic

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#### https://ngee-arctic.ornl.gov

The Arctic is a historically understudied biome that holds at least twice as much carbon as the atmosphere. Climate change and Arctic amplification are warming the Arctic faster than the rest of the world, and increasingly frequent wildfires and widespread permafrost degradation are impacting ecosystem structure and function. The Next-Generation Ecosystem Experiments (NGEE) Arctic is a model-driven, multiscale research project with a goal of improving understanding and model representation of complex interactions among climate, landforms, hydrology, biogeochemistry, vegetation, snow, and permafrost in Arctic tundra. NGEE Arctic emphasizes iterative collaboration among interdisciplinary teams of empiricists and modelers to incorporate experiments into models—underscored by open science and a safe, inclusive project culture.

Observations made by the NGEE Arctic team across a gradient of permafrost landscapes in Alaska have improved the representation of tundra processes in the Energy Exascale Earth System Model. The project's modeling approach was initially driven by the recognition that the current generation of models failed to capture many processes controlling climate feedbacks in Arctic tundra. Model improvements have emphasized unique aspects of permafrost environments and explored reductions in model complexity while retaining predictive power. The team is now leveraging Arctic-informed models to make novel predictions. For example, researchers found that improved model representation of the unique characteristics of tundra plants improved model prediction of carbon-climate feedbacks and underscored the need for dynamic vegetation. In turn, improved model representation of ground subsidence predicted that a sinking tundra surface is unlikely to trigger runaway permafrost thaw. Furthermore, machine learning algorithms trained on thousands of observations improved model representation of snow distribution across the landscape. The next phase of NGEE Arctic proposes to confront models trained on and evaluated against observations from Arctic Alaska with current observations and projected climate responses across the Arctic.

# Improvements to Land Surface Modeling in Polygonal Tundra

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For over a decade, the Next-Generation Ecosystem Experiments (NGEE) Arctic project has conducted research regarding the impact of climate change on hydrologic processes in ice wedge polygonal tundra. The long-term goal of this research is to develop process representation of changing polygonal microtopography and surface inundation dynamics within the land component of the Energy Exascale Earth System Model (E3SM), DOE's flagship Earth system model. Among the most important research questions are whether the land surface will become wetter or drier and how changes to surface wetness will impact ground-atmosphere carbon exchange. Early work focused on developing and validating the Amanzi-Advanced Terrestrial Simulator (ATS), a physics-rich surface-subsurface hydrologic code, at the spatial scale of individual ice wedge polygons. More recently, observation-constrained, basinscale Amanzi-ATS simulations on the outer coastal plain of the Beaufort Sea have projected that ice wedge polygon landscapes are likely to become drier over the next century due to improved surface drainage in thermokarst terrain. Recent satellite remote sensing work is consistent with this finding but has also demonstrated that the response of inundation dynamics will be highly impacted by macroscale topographic setting. At present, the NGEE Arctic project is conducting a new ensemble of basin-scale simulations in five watersheds throughout the Alaskan North Slope, ranging from flat to very hilly (>100 m of relief in less than 1 square kilometer). The results are being analyzed to determine new empirical relationships between surface water storage, surface inundation fraction, and runoff, which change as a function of active layer deepening to reflect the impact of ground subsidence and microtopographic deformation on surface hydrology. These new empirical equations will be embedded within the land component of E3SM and switched on within columns representing polygonal ground. This new functionality will enable regional and pan-Arctic assessments of the extent to which changing polygonal microtopography impacts Arctic carbon cycling as air temperatures continue to rise.

#### Improvements to Modeling and Predicting Snow Distribution Using Machine Learning, Physics-Based Models, and New Observational Methods

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Snowpack distribution in Arctic and alpine landscapes is highly variable and often occurs in repeating, year-to-year patterns due to local topographic, weather, and vegetation characteristics. Developing methods for monitoring and modeling complex Arctic snow distributions is key to understanding snow-vegetation interactions and subsequent impacts on permafrost. Recent advances in snow hydrology and machine learning (ML) have increased the ability to predict snowpack distribution using *in situ* observations and simple landscape characteristics (e.g., vegetation type, topographic position index, wind indices, elevation) that can be easily obtained for most environments. Here, the team presents novel methods to characterize snow-vegetation-topography interactions using ML, physics-based models, and new observational methods to determine snow depth and snow distribution in the subarctic Teller watershed on the Seward Peninsula in Alaska. First, researchers include results from a hybrid approach to couple a ML-based snow distribution pattern map with the physics-based snow process model, SnowModel. The team trained the ML algorithm on tens of thousands of snow survey observations that were collected over four winters during peak snow-water equivalent (Crumley et al. In review for Water Resources Research). The hybrid method more accurately depicted the spatial patterns seen in *in situ* observations and light detection and ranging datasets compared to SnowModel runs that did not incorporate the ML pattern map. Secondly, researchers developed a transferable ML model to predict snow depth from ground surface temperature (GST) measurements at daily temporal resolution (Bachand et al. In preparation). This model was trained on snow depth and GST data collected using distributed temperature profilers and performed well (R<sup>2</sup>>0.85) on the Seward Peninsula and elsewhere (e.g., Svalbard, Norway). These results demonstrate that ML can improve upon physics-based model results and enhance the capacity to observe snowpack characteristics in a changing Arctic environment going forward.

#### Tussock Tundra Methane Fluxes Are Heterogeneous and Sensitive to Spring Conditions: An NGEE Arctic Study at Council, AK

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Arctic tussock tundra is often treated as one plant community for modeling and projecting greenhouse gas fluxes, but small-scale heterogeneity in thaw, and thus hydrology, can have large impacts on greenhouse gas fluxes. The team measured methane  $(CH_4)$ , carbon dioxide  $(CO_2)$ , energy exchange, and above- and belowground properties between 2017 and 2023 at the Next-Generation Ecosystem Experiments Arctic site near Council, AK (AmeriFlux site US-NGC). The northern flux tower footprint was moderately dry while the southern section contained inundated thermokarst features. Thaw depth, soil moisture, and temperature were distinctively different between these sectors. While the soil thawed faster in the non-thermokarst areas in spring as thermokarst features were often covered with snow into June, by July thermokarst features reached a thaw depth of 1 m almost a month before those in the drier, upland areas. While there was little interannual variation in meteorological conditions in summer, variation in spring conditions dictated CH<sub>4</sub> fluxes at the site. The highest CH<sub>4</sub> fluxes occurred in 2019, which had a mild, wet spring (snowmelt 24 May; growing season CH<sub>4</sub> fluxes were 23.5 nanomoles per m<sup>2</sup> per second in the south, 12 nmol m<sup>-2</sup> s<sup>-1</sup> in the north). In contrast, the lowest fluxes were in 2022 when spring was cooler and drier (snowmelt 29 April; CH<sub>4</sub> fluxes were 7.8 and 4.2 nmol m<sup>-2</sup> s<sup>-1</sup> in wet and dry areas, respectively). In all years, the influence of thermokarst  $CH_4$ hot spots was clear in footprint-averaged fluxes. The areas also had different timescales of response to environmental conditions, with faster response in wet areas. Thus, tussock tundra, which is currently modeled as a single vegetation community, has highly heterogeneous CO<sub>2</sub> and CH<sub>4</sub> fluxes in space, seasonally, and interannually. These differences are associated with thermokarst and weather impacts on subsurface moisture and temperature, pointing to the need for better representation of thermohydrology in land models.

#### Thermokarsting Alters Belowground Biogeochemistry and Greenhouse Gas Fluxes

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Climate change poses a significant risk to the function of Arctic ecosystems and the stability of frozen carbon (C) currently sequestered in Arctic permafrost. Substantial progress has been made in understanding and predicting how Arctic plant and soil C cycling will respond to warming. However, models remain uncertain, particularly with respect to the variable response of soil biogeochemistry and greenhouse gas (GHG) flux to warming within different plant functional types (PFTs) and landscape positions. The project's overarching objective is to link soil GHG flux [carbon dioxide  $(CO_2)$ , methylene, nitrous oxide  $(N_2O)$ ] and soil biogeochemical variables to different landscape positions and PFTs. These findings will help resolve spatial variability in Arctic ecosystem response to warming. Here, the team presents data from field campaigns in Council, AK, in 2021 and 2023 and preliminary data from a laboratory mesocosm currently being conducted. Researchers found that a lowland thermokarst wetland containing aerenchymas graminoids acts as a net source of GHGs due to significant (p<0.05)emission of methane (CH<sub>4</sub>), while the upland tundra containing shrub, lichen, and forb PFTs generally acts as a net sink of GHGs during the late thaw season. Upland PFTs correlate well with belowground chemistry (i.e., redox, pH, dissolved organic carbon) while belowground chemistry correlates well with soil GHG fluxes ( $CO_2$ ,  $CH_4$ ,  $N_2O$ ). The project therefore postulates that PFT alters belowground biogeochemistry, which in turn affects how C is cycled and emitted as GHGs. Graminoids present at the lowland thermokarst wetland location likely contribute the most to rapid and sustained changes in belowground biogeochemistry, likely due to aerenchyma conducting GHG from the soil to the atmosphere as well as introducing oxygen to the otherwise anoxic rooting zone. The team additionally presents preliminary data on a rhizobox mesocosm experiment investigating interactions between this aerenchyma graminoid belowground biogeochemistry.

# Addressing Issues of Model Scale with New E3SM Land Model Parameterizations and a Novel Ecosystem Mapping and Modeling Approach

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Scaling is a ubiquitous challenge in Earth system models (ESMs). In the Arctic, the spatial distribution of snow depends on fine-scale processes and has impacts on underlying permafrost, regional hydrology, and ecology. Incorporating these fine-scale relationships into coarse-scale ESMs is difficult due to the challenges of accessing and observing the vast Arctic system. In this work, the project aims to improve representation of snow in the Arctic in the E3SM Land Model (ELM) through improved process representation and novel snow-scaling techniques. To improve ELM, the team leveraged and modified its existing subgrid structure and snow parameterizations. Results show that downscaling radiation and precipitation forcings based on topographic characteristics improves E3SM's snow estimates. Researchers also find that modeled vegetation heights are too tall in the Arctic. Taken together, combined with ELM's lack of wind redistribution of snow, the team finds that ELM exhibits biases in its representation of fine-scale snow processes. To complement these ELM developments, researchers propose a novel clustering technique to upscale snow characteristics from watershed to regional scales using remotely sensed landscape characteristics. This construct, which is referred to as ecosystem mapping and modeling units (EMMUs), is a promising way to infer snow distributions across large domains and to evaluate ESMs at the grid cell level (e.g., >1  $km^2$ ).

EMMUs are derived using a k-means clustering method on features derived from airborne light detection and ranging (LiDAR) data collected on Alaska's Seward Peninsula in summer 2021 and winter 2022. The team examined the relationships between snow depth and LiDAR-derived landscape characteristics to inform feature selection. The results presented include 11 clusters based on topographic position index, shrub height, and shrub density. Average snow depth differs significantly between each cluster, demonstrating that the EMMU approach could be valuable for informing and evaluating ELM developments at larger scales.

#### Improving Disturbance and Plant Functional Type Representation in ELM-FATES for Arctic Science Questions

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Shifts in Arctic vegetation are expected to continue under rapid warming, directly control ecosystem function and climate feedbacks and remain challenging to predict in ecosystem models. Therefore, the team has evaluated the role and sensitivity of the parameterization of plant functional types in model simulations at the Kougarok Hillslope site in Alaska under historical and future climates using the E3SM Land Model-Functionally Assembled Terrestrial Ecosystem Simulator (ELM-FATES). Results show that present-day modeled biomass, composition, and productivity are the most sensitive to traits controlling photosynthetic capacity, carbon allocation, allometry, and phenology. Notably, these same sets of trait configurations produce diverging biomass, composition, and productivity under future climate, where the uncertainty attributable to plant traits is twice the change attributable to climate. This larger divergence due to functional trait uncertainty motivates further work to better constrain model parameters and re-evaluate model predictions under changing climate. In addition to long-term warming, shifts in Arctic disturbance regimes will alter demographic processes of recruitment, growth, and mortality. Dynamic ecosystem modeling that includes successional demographic processes and trait-driven competitive responses to disturbance is a powerful tool to investigate these Arctic dynamics. To better understand Arctic processes under a warming climate, researchers will improve ELM-FATES to simulate the effects of wildfire disturbance on plant distribution and function and evaluate the importance of vegetation-mediated ecosystem responses in driving overall patterns of carbon cycling and greenhouse gas balance. The team presents the framework for updating ELM-FATES, including (1) an improved subgrid hierarchical framework to have modeling "columns" that reflect wildfire disturbance history, (2) differences between "evenly distributed" and "resolved" vegetation distributions in the model grid cell, (3) cross-grid seed dispersal, and (4) initial results of coupled nutrient interactions. The goal of these model developments is to link different types of rapid and heterogeneous change to explore interactions and feedbacks among them using an improved ELM-FATES.

#### Estimating Fractional Cover of Arctic Tundra Plant Functional Types on the North Slope of Alaska Using Sentinel and Harmonized Plot Observations

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Plant functional type (PFT) fractional cover (fCover) information is used to assess vegetation composition and diversity, which is crucial for understanding the health and functioning of Arctic ecosystems. Satellite data provide a means for scaling local, plot-measured fCover to regional scales. The team harmonized open-access vegetation plot data repositories that provide fCover observations in Alaska: the Alaska Vegetation Plots Database, ABR Inc.—Environmental Research and Services, the Arctic Vegetation Archive, and the National Ecological Observatory Network. Leveraging these plot datasets, researchers generated a wall-to-wall map of fCover for tundra PFTs on the north slope of Alaska. While the plot fCover provide invaluable information about the tundra vegetation, they contain large inconsistencies in terms of sampling scale (species- or PFT-level), plot size (0.5 to 55 m in radius), collection year (1950 to 2021), field sampling approaches (point- or quadrat-intercept), and fCover measurement (percent or Braun-Blanquet codes). The team harmonized the plot fCover using a consistent PFT schema: nonvascular, forb, graminoid, deciduous shrub, evergreen shrub, and two non-PFT classes (bare ground and water, suitable for parameterizing terrestrial land surface models). Researchers then linked the plot fCover with satellite-derived explanatory variables (Sentinel-2 spectra, phenology, and Sentinel-1 polarization bands) and trained random forest regression models to estimate fCover. To reduce the spatiotemporal inconsistencies between plot and satellite observations, the team adopted a multivariate outlier detection approach-Cook's distance—to identify high-quality plots for model training and validation. The results suggest that the random forest regression models can estimate fCover with good accuracy. The correlations between plot-observed and satellite-derived fCover are substantially improved when using high-quality plot samples. The mapped fCover characterizes the spatial patterns of different PFTs across the tundra biome at a high resolution, providing information needed for improved representation of Arctic tundra vegetation in Earth system models to better quantify climate-vegetation feedbacks in the Arctic tundra ecosystem.

#### **Impacts of Wildfire on Arctic Shrub Expansion**

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Northern high-latitude regions have experienced rapid warming and more frequent and intense wildfire in recent decades. These changes contribute to a complex set of soil-plant-atmosphere interactions, potentially altering competitive interactions, plant species composition and abundance, and ecosystem carbon stocks. Increases in woody plants, particularly tall deciduous shrubs, have been observed across much of the Arctic tundra region. However, the role wildfire plays on observed shrub expansion is uncertain. Here, the team applied a process-rich ecosystem model, *ecosys*, to examine changes in tundra shrub growth driven by wildfire across Alaska.

After thoroughly evaluating model simulations against site observations and data-driven regional products, researchers found that the impact of wildfire on Arctic shrub growth is spatially heterogeneous. The team modeled that changes in soil moisture postfire are a key factor that controls successful establishment and relative competitiveness of shrubs. Fire generally enhances the growth of shrubs in areas that are sufficiently drained and have optimal soil moisture versus in areas with postfire saturated conditions. The project shows that postfire deepening of the active layer, driven by warmer soil, accelerates nutrient cycling. Further, changes in soil moisture regime control trajectories of shrub growth and their ability to compete with herbaceous plants under increased wildfire and climate warming.

# Arctic Ecosystem Modeling: What Role Can Paleo History Play in Reducing Model Uncertainty?

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Ongoing and expected changes in the carbon balance of the Arctic tundra are important for the global carbon budget, but uncertainty remains in the ability to model Arctic ecosystems. The influence of initial conditions is often underestimated as a source of this model uncertainty, particularly with respect to the initial model set-up with pre-run, equilibrium, and spin-up simulations that are necessary to reach an accurate representation of pre-industrial conditions. This is particularly relevant in areas underlain by permafrost like the Arctic.

Arctic permafrost contains large amounts of carbon (1,460 to 1,600 petagrams of carbon) and dates to the last glacial maximum (LGM). This permafrost has remained stable under pre-industrial conditions due to a hysteresis behavior, resulting in a much longer thermal memory than commonly accounted for in modeling. Consequently, this leads to an underestimation of pre-industrial permafrost extent and may cause significant model uncertainty concerning carbon balance and soil temperatures.

The project assesses whether considering paleo history improves soil thermal and carbon balance representation in the Dynamic Vegetation, Dynamic Organic Soil, Terrestrial Ecosystem Model. Researchers conduct simulations at several sites across Alaska and compare simulations with and without paleo history with borehole observations and carbon flux measurements. The team examines the impact of different paleo climate scenarios, each varying the temperature difference from the LGM to pre-industrial conditions. Initial simulations reveal that colder paleo climate scenarios result in initially cooler soils, which in some instances exhibit a more rapid warming trend under recent climatic warming compared to warmer scenarios. This shift in thermal dynamics carries significant implications for the carbon balance and overall model uncertainty. Through this project, the team aims to assess the potential benefits of adopting paleo history more widely in modeling to reduce these model uncertainties.

# Incorporation of Diverse Arctic Vegetation Types in a Land Surface Model Improves Representation of Spatial Variability in Carbon Dynamics Across a Tundra Landscape

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Earth system models (ESMs), particularly land surface components that simulate complex interactions between vegetation and the atmosphere, serve as essential tools for comprehending climate change. The Arctic is experiencing warming trends surpassing those observed elsewhere on Earth. Given the considerable carbon stored in permafrost that is susceptible to release with ongoing warming, permafrost thaw has the potential to significantly impact global carbon cycling and ecosystem-climate feedbacks. However, model predictions of climate change in Arctic regions are uncertain, in part due to challenges in capturing the complexity of Arctic ecosystems and the historically limited availability of observational data for model validation and calibration. Arctic ecosystems are typically represented in a highly simplified manner. For instance, the Energy Exascale Earth System Model (E3SM) divides Arctic vegetation into two plant functional types (PFTs): deciduous shrub or grass. Recent efforts have integrated diverse Arctic PFTs into the E3SM Land Model (ELM), leveraging the wealth of data from the Next-Generation Ecosystem Experiments (NGEE) Arctic to parameterize the additional PFTs. In this study, researchers conducted spatially explicit  $100 \times 100$  m resolution simulations of vegetation and associated carbon dynamics at the NGEE Arctic Council study site on Alaska's Seward Peninsula, using ELM configured with the improved representation of Arctic vegetation.

Comparison of model predictions with observational data (e.g., eddy covariance flux tower, airborne hyperspectral remote sensing, and machine learning–based plant community characterization) reveals that the refined PFT representation produced more realistic spatial patterns of tundra vegetation biomass and land-atmosphere exchanges compared to the original model. Variability in vegetation biomass and productivity across the tundra landscape was much higher when incorporating multiple tundra plant growth forms. Results demonstrate that enhanced model representation of the diversity of Arctic vegetation can provide a more robust predictive understanding of carbon dynamics across tundra landscapes, facilitating regional to pan-Arctic scaling.

### Unraveling the Impacts of Snowpack Dynamics, Soil Properties, and Near-Surface Hydrology on Soil Temperatures and Biogeochemical Processes in Two Discontinuous Permafrost Watersheds

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In high-latitude permafrost environments, snowpack dynamics, soil properties, and near-surface hydrology are linked with soil thermal regimes, vegetation dynamics, and carbon cycling. Better understanding of these links requires collection of spatially and temporally dense hydrogeochemical data, which is made challenging by remote field locations and harsh environmental conditions. Here, the project uses spatially and temporally dense measurements of snowpack dynamics and soil temperature in conjunction with model experiments to explore the connections between snow, water, and carbon in two discontinuous permafrost watersheds.

The team collected co-located, vertically resolved time series of snow and soil temperature every 5 or 10 cm along 1.2 or 1.6 m probes between June 2021 and September 2023 at 82 locations in the Teller 27 watershed and 44 locations in the Kougarok watershed on the Seward Peninsula in Alaska. Researchers further perform one-dimensional model experiments using *ecosys*, a mechanistic, process-rich ecosystem model that has been successfully tested across high latitudes.

Variation in annual maximum snow depth is strongly correlated with mean annual soil temperatures at both sites. Researchers also find that interannual variability in snow regimes drives interannual variability in near-surface soil temperatures during the growing season. Modeled and observed snowpack dynamics (snow depths and snow temperature profiles) closely match observations throughout both years of data. A model sensitivity analysis shows that, in addition to snow depth, soil thermal-hydrological characteristics have a strong impact on simulated soil temperatures. This model result is used to explain why locations with similar snow depths can have different soil thermal regimes. The team further finds that spatial variation in snow depths is associated with variation in rates of biogeochemical processes (e.g., more primary productivity in areas of deep snow), and that interannual variation in snowmelt timing has a strong impact on growing season dynamics (e.g., leaf out date and growing season length).

#### Simulating Arctic Soil Redox and Biogeochemical Interactions in the E3SM Land Model

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Redox cycles, geochemistry, and pH are recognized as key drivers of subsurface biogeochemical cycling in terrestrial and wetland ecosystems but are typically not included in terrestrial carbon cycle models. These omissions may introduce errors when simulating carbon cycling and greenhouse gas emissions in systems where redox interactions and pH fluctuations are important, such as wetland-rich tundra landscapes where saturated soil conditions combined with high soil iron concentrations can influence biogeochemistry. The project coupled the E3SM Land Model (ELM) with geochemical reaction network simulator PFLOTRAN, allowing geochemical processes and redox interactions to be integrated with land surface model simulations. Researchers implemented a reaction network including aerobic decomposition, fermentation, iron oxide reductive dissolution and dissolved iron oxidation, and methanogenesis as well as pH dynamics. The team used the model framework to simulate biogeochemical cycling and methane production across tundra landforms including permafrost polygons and thermokarst features. Model simulations were parameterized using laboratory incubations and compared well with measured porewater concentrations and surface gas emissions from Next-Generation Ecosystem Experiments Arctic field sites. These results demonstrate how directly simulating biogeochemical reaction networks can improve land surface model simulations of subsurface biogeochemistry and carbon cycling in tundra ecosystems.

# Metagenomics and Synchrotron Fourier Transform Infrared Resolved Changes in Carbon and Nitrogen Cycling in an Arctic Tundra

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This project uses state-of-the-art sequencing and imaging technologies to resolve complex interactions governing biochemical cycles in tundra biomes to inform efforts to decipher Arctic carbon and nitrogen cycling. Arctic soils are crucial in climate change research due to potential rapid microbial mineralization and increased greenhouse gas (GHG) emissions under rising temperatures. The diverse microbial habitats in these soils, shaped by various landscape features, show varying responses to warming, but the seasonal impact on GHG production remains unclear. Between 2011 and 2022, the team conducted multiple sampling campaigns to collect active layer soils from the polygonal Arctic tundra at the Barrow Environmental Observatory. Researchers analyzed these soils' chemical and biological properties and performed lab-scale soil incubations to test the impact of warmer winters on GHG emissions. To better understand the microbial communities in these soils, the team extracted and sequenced the whole community DNA and reconstructed prokaryotic and viral genomes. In addition, researchers analyzed the soil biochemistry via synchrotron Fourier transform infrared spectral imaging at the Berkeley Infrared Structural Biology beamline of the Advanced Light Source to link soil chemistry and microbial communities. The team discovered that the microbiomes are organized by topography, significantly influencing the distribution of genes linked to GHG emissions, with GHG production potential varying across different polygons. At the site, limited pools of butyrate, lactate, formate, and acetate were observed with carbon chemistry predominantly consisting of lignocellulose and chitin where microbes were mostly found.

Marginal differences in the distribution of carbon compounds between organic and mineral layers were detected, paralleling genomic data observations. Especially in wetter portions of the landscape, significantly higher carbon dioxide fluxes were detected after a warm winter. The project's research highlights that landscape topography primarily determines microbial functions, and integrating these with geochemistry and GHG fluxes offers insights into Arctic soil biogeochemical cycles.

# Using Machine Learning to Estimate Near-Surface Permafrost Extent at NGEE Arctic Sites on the Seward Peninsula in Alaska

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Permafrost soils are a critical component of the global carbon cycle and are locally important regulators of hydrologic fluxes from uplands to rivers. Furthermore, degradation of permafrost soils can lead to land surface subsidence, damaging crucial infrastructure for local communities. Regional and hemispherical maps of permafrost are too coarse to resolve distributions at a scale relevant to assessments of infrastructure stability or to illuminate geomorphic impacts of permafrost thaw. Here, researchers train machine learning models to generate meter-scale maps of near-surface permafrost for three watersheds in the discontinuous permafrost region. The models were trained using ground truth determinations of near-surface permafrost presence from measurements of soil temperature and electrical resistivity. The team trained three classifiers: extremely randomized trees (ERTr), support vector machines (SVM), and an artificial neural network (ANN). Model uncertainty was determined using k-fold cross validation, and the modeled extents of near-surface permafrost were compared to the observed extents at each site. At-a-site near-surface permafrost distributions predicted by the ERTr produced the highest accuracy (70 to 90%). However, the transferability of the ERTr to sites outside of the training data set was poor, with accuracies ranging from 50 to 77%. The SVM and ANN models had lower accuracies for at-a-site prediction (70 to 83%), yet they had greater accuracy when transferred to the nontraining site (62 to 78%). These models demonstrate the potential for integrating high-resolution spatial data and machine learning models to develop maps of near-surface permafrost extent at resolutions fine enough to assess infrastructure vulnerability and landscape morphology influenced by permafrost thaw. However, transferrable machine learning models for estimating near-surface permafrost extent across ecosystems and disturbances histories will require additional ground truth datasets, which are currently underdeveloped.

# A Managed Project Data Space that Supports a Proposed NGEE Arctic Phase 4 Integrated ModEx Framework

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This project describes how researchers will support data collections and management of a proposed Next-Generation Ecosystem Experiments (NGEE) Arctic Phase 4 to allow for coordinated data use among an interdisciplinary team of empiricists and modelers, as well as how the team will continue to provide a foundation of open science and data sharing through an NGEE Arctic Managed Project Data Space.

The NGEE Arctic Data Management Team (DMT) recognizes the need for coordinating a collection of baseline datasets that support the modeling activities of three proposed Phase 4 model-experiment questions and three proposed Phase 4 crosscut science activities. These datasets range widely from synthesized model evaluation site data to regional and pan-Arctic initialization, parameterization, and evaluation data. Scaling activities will determine NGEE Arctic data standards, ensuring coordination of research activities and facilitating data interoperability. The DMT will create and foster a Managed Project Data Space and an associated data catalog that will be a compute resource providing open and shared access to an organized collection of datasets. Phase 4 Science Teams will both contribute to and access these organized data thereby ensuring data coordination across modeling activities, reducing duplication of effort, mitigating model uncertainties, and fostering consistent workflows. This compute and data access resource will be an allocation of Oak Ridge National Laboratory's (ORNL) Scalable High Performance Computing Condo known as the Compute and Data Environment for Science (CADES). CADES' Open Protection Zone allows researchers inside and outside of ORNL access to dedicated infrastructure, sustained storage and access, compute resources, and customizable software as a service. The DMT will develop the infrastructure and manage a data catalog that allows easily searchable high-level metadata for site, regional, and pan-Arctic datasets and provides contextual information of spatial and temporal extents and resolutions of data. The DMT will assist Phase 4 researchers with publishing all mature datasets into DOE's Environmental System Science Data Infrastructure for a Virtual Ecosystem long-term repository.

#### Multiscale Modeling and Model-Data Integration to Improve the E3SM Land Model

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The overarching objective for the Next-Generation Ecosystem Experiments (NGEE) Arctic project is to deliver an improved predictive understanding of Arctic tundra processes at the scale of a high-resolution Earth system model (ESM) grid cell. To achieve that goal, the team has identified six Integrated Modeling efforts, each of which results in improved prediction capability implemented within DOE's Energy Exascale Earth System Model (E3SM). During Phase 3 of NGEE Arctic, researchers are synthesizing observations, experiments, and fine-scale modeling results to arrive at new E3SM Land Model (ELM) parameterizations suitable for a high-resolution ESM grid cell. Over the past year, the team has made significant progress in connecting high-resolution and process-resolving simulations to sitescale observations to improve understanding of fundamental controls on hydrologic, thermal, and biogeochemical processes in Arctic tundra landscapes. Researchers have also made important advances in developing new process parameterizations and designing new implementations of subgrid process heterogeneity to migrate new knowledge from finescale simulations into improvements in ELM. Here, the team shows examples of improvements in ELM from studies of subgrid fractional area of inundation, hydrologic coupling across subgrid hillslope elements, snow-vegetation interactions in complex topographic settings, complex and dynamic vegetation communities, and redox-resolving biogeochemical reaction networks.

The project draws connections from lessons learned in the NGEE Arctic project to other studies in different ecosystems. The team shows examples of connections between Arctic tundra and coastal wetland systems, focusing on improved representation of processes such as redox-enabled biogeochemistry and improved treatment of subgrid heterogeneity in complex ecosystems with small-scale variation in structure and function.

# E3SM Land Model Simulated Snow Seasonality in NGEE Arctic's Alaskan Seward Peninsula Study Region Affected by Topography, Plant Functional Types, and Meteorological Forcings

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In the Arctic, snow processes are of great challenge in Earth system models, especially in highly heterogeneous areas like the Alaskan Seward Peninsula where there is a lack of reliable input data consistent in both space and time series. In this study, the team presents some initial high-resolution  $(1 \text{ km} \times 1 \text{ km})$  land-surface modeling results in that region using the E3SM Land Model (ELM) and data collected by or for the Next-Generation Ecosystem Experiments Arctic project.

Researchers integrated a few high-resolution surface properties for the region, including: (1) a newly developed tundra plant functional type dataset, derived from field investigations and remote sensing, with field-based model development and parameterizations (Sulman et al. 2021); (2) topography derived from the Arctic Digital Elevation Model (https://www.pgc.umn.edu/data/arcticdem/); (3) soil thickness (https://daac.ornl.gov/SOILS/guides/ Global\_Soil\_Regolith\_Sediment.html); and (4) soil physical properties (https://soilgrids.org). The model is driven by three forcing datasets: half-degree resolution Global Soil Wetness Project Phase 3 (GSWP3) Version 2, half-degree resolution CRU-JRAS v2.3, and 1 km×1 km GSWP3-Daymet (https://daymet.ornl.gov).

The preliminary data analysis in general shows reasonable and more realistic snow coverage on the ground and snow-free seasonality compared to a global high-resolution dataset of snow coverage from the U.S. National Ice Center Ice Mapping System (https://usicecenter.gov/Resources/ ImsInfo). Those improvements are associated with detailed topography, soil, and vegetation features, even with coarse forcings. The 1-km resolution Daymet forcing can further improve the modeled snow distribution pattern in terrain. Further improvement of snow fence effects in tall shrubby land would be another critical step for ELM modeling in high-latitude regions.

### Evaluation of Earth System Model Simulation for Subsurface Thermal Dynamics of Arctic Landscapes: Insight from an Intermodal Comparison at a Column Scale

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The Arctic is warming twice as fast as the rest of the planet, which poses a significant threat to both the Arctic and low-latitude regions. Earth system models (ESMs) serve as efficient tools for capturing interactions and predicting the impacts of Arctic warming. Within an ESM, the land model component is critical for simulating hydrothermal, ecological, and biogeochemical processes. Many ESM-based studies focus on Arctic prediction by improving process representation and employing finer mesh resolutions. However, the uncertainties of these model predictions are still poorly understood due to of a lack of observations that can be used for comparison at ESM scales. To address this, the study explores a novel model-data integrated approach (ModEx) to evaluate ESM predictions for Arctic landscapes. The team focused on the performance and uncertainty in DOE's E3SM Land Model (ELM) in simulating subsurface hydrothermal dynamics for tundra landscapes. Using the field observations and well-tested process-based Advanced Terrestrial Simulator (ATS) model at the Barrow Environmental Observatory (BEO) as a reference, researchers validated ELM's simulation for the BEO site at a column scale. Using the same parameters, subsurface layer partitioning, and meteorological forcing in ELM and ATS, the team found that ELM, with its default 15% soil moisture as the initial condition, consistently underestimates soil moisture. However, aligning with the ATS initialization strategy of using saturated soil as an initial condition, ELM significantly improves in modeling soil moisture variation. Adopting this initialization approach, subsequent simulations found that the ELM subsurface temperature fits well with field observations. The project's simulations also found that snow is an important control on ELM subsurface simulation. The study showcases the effectiveness of the ModEx approach to evaluate ESM performance in Arctic prediction with the potential to extend this approach to evaluate other processes beyond subsurface hydrothermal dynamics.

# Next-Generation Ecosystem Experiments Tropics

# Next-Generation Ecosystem Experiments (NGEE) Tropics Phase 2 Overview

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Tropical forests exchange more carbon dioxide, water, and energy with the atmosphere than any other biome. Yet processes controlling tropical forest-atmosphere interactions that play key roles in regulating Earth's climate are not well represented in the current generation of Earth system models. In support of BER's mission to advance a predictive understanding of Earth's climate and environmental systems, the goal of the Next-Generation Ecosystem Experiments (NGEE) Tropics project is a greatly improved predictive understanding of tropical forests and Earth system feedbacks to changing environmental drivers over the 21st century. A strong coupling of modeling and experiment-observational methods (ModEx) is the fundamental approach toward attaining this goal, with a grand deliverable of a representative, process-rich tropical forest ecosystem model (Functionally Assembled Terrestrial Ecosystem Simulator; FATES), where the dynamics and feedbacks of tropical ecosystems in a changing climate are modeled at the scale and resolution of a next-generation Energy Exascale Earth System Model (E3SM) grid cell. The current Phase 2 of NGEE Tropics is structured around three Research Focus Areas (RFAs) that will advance understanding and model representation of tropical forest processes at individual (RFA1), community to regional (RFA2), and regional and global (RFA3) scales in E3SM-FATES. Science activities within these RFAs are organized into ModEx Work Packages (WP). This overview will highlight activities that synthesize across RFAs and WPs toward addressing integrative science questions at site to continental scales.

# Advancing Model Predictions of Tropical Forest Response to Droughts

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In a demonstration of model-experiment (ModEx) success, the Next-Generation Ecosystem Experiments (NGEE) Tropics project is using diverse co-located datasets to advance understanding of tropical forest function and the predictive ability of global vegetation models. For example, via a complex data-model integration in Panama, the team found that if vegetation demography models (VDMs) are to correctly represent drought resilience of tropical forests, they must account for trees' rooting depths (drought avoidance) and not merely hydraulic vulnerability traits (drought resistance). Researchers found that deeper-rooted tree species were more hydraulically vulnerable but survived through several droughts compared to shallow-rooted trees. Thus, without accounting for rooting depths, VDMs would kill the wrong plant functional types, leading to misleading predictions of changes in forest function.

The large set of co-located measurements collected by NGEE Tropics—from hydrology and tree demography to water-sourcing depths, hydraulic traits, and other carbon- and water-related responses across sites in Brazil and Panama—are being used for DOE's E3SM–Functionally Assembled Terrestrial Ecosystem Simulator (E3SM-FATES; -Hydro) model improvements. Here, the team summarizes current and planned hypotheses tests to quantify wholeplant drought resilience strategies and their coordination with other stress axes (light, nutrients, heat, fire) across representative pantropical forest communities along climatic, edaphic, water table, and disturbance gradients. This will enable representation of the true diversity and resilience of tropical forest response and feedback to carbon dioxide, climatic, and land-use change in E3SM.

# Spatial and Temporal Drivers of Tropical Forest Canopy Disturbances from Annual Drone Photogrammetry

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Disturbance rates are an important control over variation in tropical forest carbon stocks and fluxes. However, there is much uncertainty regarding the relative importance of potential drivers of disturbance rate variation in space and in time. In previous Next-Generation Ecosystem Experiments (NGEE) Tropics research, the team used repeat drone photogrammetry to demonstrate that disturbance rates varied over threefold spatially within the landscape of Barro Colorado Island in Panama (Cushman et al. 2022). Soil type, forest age, and topography explained approximately half of this spatial variation, with important consequences for standing carbon stocks across the landscape. Here, researchers extend previous analysis to explore whether the spatial patterns found in Cushman et al. are consistent over time, using an updated dataset of six annual drone surveys from 2018 to 2023 with improved georeferencing from recent airborne light detection and ranging data. The team also explores whether interannual variation in disturbance rates are related to patterns of convective available potential energy (CAPE) associated with mesoscale convective systems or locally measured precipitation events. Other NGEE Tropics research has shown the importance of CAPE for large windthrows across the Amazon basin (Feng et al. 2023). This project combines these areas of interest within NGEE Tropics to characterize disturbance dynamics in tropical forests.

Cushman, K. C., et al. 2022. "Soils and Topography Control Natural Disturbance Rates and Thereby Forest Structure in a Lowland Tropical Landscape," *Ecology Letters* **25**(5), 1126–38.

Feng, Y., et al. 2023. "Amazon Windthrow Disturbances Are Likely to Increase with Storm Frequency Under Global Warming," *Nature Communications* **14**(1), 101.

# Towards Amazon Basin-Scale Vegetation-Hydrology Modeling Using ELM-ParFlow-FATES

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Moderated by topography, climate change is likely to cause large and diverse impacts on plant water availability, with consequential impacts on vegetation dynamics and water cycle processes. The project has developed an integrated model, ELM-ParFlow-FATES, which couples the E3SM Land Model (ELM), an ecosystem dynamics model (Functionally Assembled Terrestrial Ecosystem Simulator; FATES), and a three-dimensional hydrology model (ParFlow) to explicitly resolve hillslope topography and subsurface flow for better understanding of the processes that drive plant water availability and tropical forest dynamics. Numerical simulations of 1-km resolution are conducted using ELM-ParFlow-FATES at the Amazon basin, leveraging high-resolution hydraulic parameter maps for surface soils and 1 km land surface dataset in tropical South America. Four types of tropical trees that are dominant in the Amazon are simulated in the model using the FATES-SP mode. The model results are being evaluated using highly resolved hydrological and vegetation data retrieved from the new generation of satellite missions. Analysis is also being performed to understand water storage, vegetation water sourcing along hillslope gradients, and vegetation response to flood and drought. Numerical experiments will then be performed using ELM-ParFlow-FATES to answer questions of how dynamic structure and biomass of different vegetations in Amazon respond to climate change.

# Accelerated Daytime Stem Growth and Respiration of Canopy Trees in the Amazon Basin

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Tropical forests cycle a large amount of carbon dioxide (CO<sub>2</sub>) between the land and atmosphere with a substantial portion of the return flux due to tree respiratory processes. However, due to the lack of a commercial real-time stem  $CO_2$  efflux (E<sub>s</sub>) system, *in situ* quantification of woody tissue respiratory fluxes remains limited in tropical ecosystems, with little information available on the interacting roles of plant biophysical (wood density and size), physiological (transpiration and growth rates), and environmental (temperature and vapor pressure deficit) factors. In this study, the team hypothesizes that fast-growing tree species with low wood density will have higher respiratory fluxes compared with slower-growing tree species with higher wood density but stem radial growth and its associated respiratory production of  $CO_2$  is highly sensitive to declines in turgor pressure associated with transpiration. Using custom systems for real-time stem E<sub>s</sub> observations, researchers quantified diurnal E<sub>s</sub> patterns in the BIONTE experimental tropical forest site near Manaus, Brazil. Researchers synthesize diurnal E<sub>s</sub> observations over 24 hours from 32 tree species during the 2022 dry and 2022 to 2023 wet seasons. In addition, the team presents a combined analysis of 5- to 7-day continuous observations of E<sub>s</sub>, sap velocity and stem water potential during the 2023 dry and 2024 wet seasons as well as vertical gradients in stem E<sub>s</sub> for a limited number of species. The observations are presented as a Next-Generation Ecosystem Experiments Tropics data archive and compared with Functionally Assembled Terrestrial Ecosystem Simulator model simulations of maintenance and growth respiration rates.

#### Integrating Global Land-Use Change Drivers into ELM-FATES

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The vegetation demographic model E3SM Land Model-Functionally Assembled Terrestrial Ecosystem Simulator (ELM-FATES) allows for the representation of disturbance processes and their legacies through a patch-based representation of subgrid-scale disturbance history. The project has extended the prior representation of natural disturbance and anthropogenic logging activities to include a generalized representation of natural and anthropogenic land use disturbance. The team leverages the patch concept in the model to include both continuous (age since last disturbance) and categorical (land use type; optionally plant functional type if prescribing land cover) variables. Land use types currently include primary lands, secondary lands, rangelands, pastures, and croplands. The model is driven directly by global historical and scenario-dependent future land-use states and transitions from the Land-Use Harmonization 2 dataset, which sets initial amounts, drives dynamic changes to land use type areas, and updates land cover. Land cover changes in the model respond to land use change in the driver datasets either through management activities (if prognosing land cover) or through a spatially resolved, time-independent land use to plant functional type correspondence dataset based on remote sensing data (if prescribing land cover). The one-way conversion of land use from primary to secondary land from logging, as well as the resolved legacies of land use, require a different approach to model initialization than is used in non-demographic models. The team will present model design, initialization strategies, and initial results.

# Exploring the Relative Role of Vapor Pressure Deficit and Soil Moisture on Vegetation Productivity Using Data-Driven Machine Learning

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With increasing frequency and severity of droughts projected for the future climate with warming, the impact of drought on vegetation productivity is expected to intensify. Drought stress on ecosystem productivity is commonly characterized by low soil moisture (SM) and high atmospheric water demand (i.e., high vapor pressure deficit; VPD). However, the relative dominance of VPD versus SM on vegetation production is still being debated. In this study, the team presents an explainable machine-learning approach to disentangle the relative role of VPD and SM on vegetation greenness (i.e., normalized difference vegetation index) across global ecosystems with a particular focus on tropical regions such as the Amazon basin using multisource datasets. The project's research shows that globally, SM typically has a more pronounced effect on vegetation greenness variation than VPD in most regions. However, in tropical forests, VPD is the more critical factor compared to SM. The relative importance of VPD and SM varies with climate and plant functional types. The study provides a large-scale benchmark for modeling the drought impacts on terrestrial ecosystems in Earth system models like DOE's Energy Exascale Earth System Model with vital implications for understanding global water, carbon, and energy cycles in the face of climate change.

#### Regional-Scale, Observation-Informed Tropical Forest Diversity in ELM-FATES

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#### https://ngee-tropics.lbl.gov

Droughts in tropical ecosystems are increasingly hotter and more frequent, with potentially significant impacts on carbon and water cycles throughout the 21st century. The ability to predict how forests will respond to climate change will largely depend on whether terrestrial biosphere models represent the diversity of individual trees' trade-offs between allocation of resources to growth and drought tolerance. Here, the project presents its approach to define regional-scale plant functional types (PFTs) for the Functionally Assembled Terrestrial Ecosystem Simulator (FATES). The team pooled trait and allometry data from multiple open-source databases (including TRY and Environmental System Science Data Infrastructure for a Virtual Ecosystem) of 34 traits across 2,096 tree species in the Neotropics and used an unsupervised clustering approach to identify and implement PFTs along the main observed trade-off axes. This approach generated five tropical PFTs (four evergreen, one drought-deciduous), with the evergreen clusters representing structural growth strategies (maximum height), tolerance to shade, and leaf stoichiometry. The team tested FATES at multiple mature forest sites along a precipitation gradient (500 to 3,000 millimeters per year) in the Neotropics. Researchers found that FATES qualitatively represents biomass differences across dry and moist forests but overestimates drought-deciduous abundance and underestimates evergreen PFT fractions under current climate. The project is currently implementing a multisite parameter sensitivity to further constrain the model predictions. Results hitherto indicate a potential for advancing understanding of PFT co-existence across the tropics using observed traits;

however, they suggest that additional data and model process development are needed to quantitatively improve the model predictions.

#### The Past and Future of NGEE Tropics Measurements and ModEx

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#### https://ngee-tropics.lbl.gov

Next-Generation Ecosystem Experiments (NGEE) Tropics has promoted leaps forward in understanding of tropical tree function from root to global scales using deliberate integration of empirical and numerical approaches. The empirical work has tested numerous hypotheses regarding tropical tree function at the site level, the data of which are being employed for model development. Functionally Assembled Terrestrial Ecosystem Simulator (FATES) efforts have simultaneously resulted in large advances in mechanistic representation of forest function. One critical next step is to emphasize efforts on model-experiment (ModEx) hypotheses from tissue to pantropical scales. To test FATES's capability to simulate physiological and demographic processes, the model will be evaluated at five sites located across Malaysia, Panama, and Brazil, where extensive water- and carbon-related traits and processes are being measured at root to whole-tree scales. These simulations allow rigorous evaluation if the model gets the right answers for the right reasons and simultaneously allows tests of alternative mechanisms underlying variation in carbon and water fluxes and demography. At the pantropical scale, the team is utilizing long-term networks of forest demographics, carbon storage, nutrient availability, and functional traits to provide the basis for empirical and numerical hypotheses. Finally, remotely sensed datasets are being used for model parameterization of biomass, wind disturbance, and land use at large scales. Here, the team summarizes the existing

and planned datasets, model developments, and associated ModEx efforts and highlights the key next steps to achieve the goal of generating a process-rich model that accounts for carbon dioxide, climate, and land-use impacts on the pantropical carbon sink.

#### Soil Nutrient Controls on Biomass Productivity Across Lowland Tropical Forests

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The future capacity of tropical forests to sequester carbon remains uncertain, partly due to the diverse nutrient requirements of trees [e.g., nitrogen, potassium, calcium, phosphorus (P), and magnesium] beyond carbon for their growth. Additionally, tropical forests exhibit considerable soil fertility variation, resulting in a heterogeneous spatial distribution of trees with diverse species, sizes, ages, and ecological functions. Consequently, the responses of tree growth and overall biomass accumulation may not be consistent across different forests or even within the same forest. The project addresses a fundamental yet crucial hypothesis aimed at understanding the role of nutrients in regulating forest productivity. Specifically, the team posits that trees situated in exposed canopy positions show a more pronounced response to nutrient limitations compared to their counterparts in shaded areas. To test this hypothesis, researchers assessed the association between aboveground woody biomass productivity and soil nutrients, focusing particularly on soil P, across eight lowland tropical forests. The team found that across all canopy levels, there is no consistent association between mean aboveground biomass accumulation and soil P among and within these eight sites, except one site (Lambir in Borneo). However, across the eight sites, aboveground biomass accumulation in the upper canopy layers tends to increase with increasing soil P. In contrast, the understory layers do not respond to soil P changes. The response of biomass accumulation to nutrient limitations is not uniform among and within forests.

Specifically, aboveground biomass accumulation is P-limited, particularly in exposed canopy positions. This is attributed to the higher productivity of canopy plants with increased access to light, more nutrient requirements for rapid tissue growth, and heightened respiration rates. Conversely, understory plants experiencing limited light availability exhibit reduced growth and nutrient requirements due to a lower carbon supply for tissue development.

# Vertical Scaling of Leaf Maintenance Respiration Through the Canopy Influences Individual Tree Carbon Budgets with Consequences for Forest Leaf Area and Biomass

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#### https://ngee-tropics.lbl.gov

The balance between respiration and photosynthesis influences the carbon budget of individual plants, with consequences for ecosystem biomass and leaf area. Photosynthesis decreases with light attenuation through the canopy, but it is less well understood how leaf maintenance respiration  $(R_{dark})$  scales through the canopy. Recent observations from a tropical forest in Panama suggest that decreases in R<sub>dark</sub> may be greater than decreases in photosynthesis. Here, the project uses the Functionally Assembled Terrestrial Ecosystem Simulator (FATES) with the E3SM Land Model (ELM) to test the sensitivity of ecosystem dynamics to the vertical scaling of  $R_{\text{dark}}$ . In pantropical simulations, researchers alter the parameter k which controls the shape of the negative exponential describing the decrease in  $R_{dark}$  with canopy depth. The team compares simulations to a control simulation where photosynthesis and respiration are proportional through the canopy. Simulations with k decreased by 0.75, corresponding to  $R_{dark}$ approximately 40% lower at the bottom of the canopy, have annual understory mortality rates approximately 1.5% lower than the control. In FATES, plants dynamically adjust their target allometric leaf biomass to prevent leaf layers with a negative carbon budget, and this trimming is decreased with decreased  $R_{dark}$ . As a result of both increased understory survival and reductions in trimming, decreased R<sub>dark</sub> results in a 21% increase in leaf area and a 12% increase in total vegetation biomass. Next-generation vegetation demographic models with multiple canopy layers must correctly represent the vertical scaling of photosynthesis and respiration through the canopy. Further observations from a diversity of sites and plant functional types could help to constrain this important process.

#### CMIP6 HighResMIP Bias in Extreme Rainfall Drives Underestimation of Amazonian Precipitation

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Extreme rainfall events drive the amount and spatial distribution of rainfall in the Amazon and are a key driver of forest dynamics across the basin. This study investigates how the 3-hourly predictions from 17 models in the High-Resolution Model Intercomparison Project (HighResMIP, a component of the recent Coupled Model Intercomparison Project Phase 6) represent extreme rainfall events at annual, seasonal, and subdaily time scales. Tropical Rainfall Measuring Mission (TRMM 3B42) 3-hour data were used as observations. Eleven HighResMIP models showed the observed association between rainfall and number of extreme events at the annual and seasonal scales. Two models captured the spatial pattern of number of extreme events at the seasonal and annual scales better (higher r values) than the other models. None of the models captured the subdaily timing of extreme rainfall, though some reproduced daily totals. Therefore, higher model resolution may be necessary but not sufficient to accurately reproduce the number and time of extreme rainfall events in the Amazon. Improving the representation of Amazon extreme rainfall events in HighResMIP models can help reduce model rainfall biases and uncertainties and enable more reliable assessments of the water cycle and forest dynamics in the Amazon.

#### Regulation of Whole-Tree Crown Conductance in Tropical Forests Across a Steep Climatic Gradient

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#### https://ngee-tropics.lbl.gov

Transpiration is strongly regulated by crown conductance but the mechanisms underlying variation in crown conductance are poorly understood in hyper-diverse tropical wet forests. Understanding this regulation is key to prediction of tree responses to climate changes. The team tested hypotheses regarding functional trait and environmental impacts on crown conductance at three forests across a moisture gradient in Panama. Crown conductance and its sensitivity to vapor pressure deficit (VPD) were among the highest ever measured globally.

Location along the moisture gradient, leaf phenology, and shade tolerance were not good predictors of transpiration or crown conductance. Trees from all three sites exhibited consistent responses of crown conductance and its sensitivity to VPD to soil moisture content but were less responsive to other climate variables. Similarly, crown conductance increased strongly with the degree of anisohydry. However, crown conductance response to whole-tree hydraulic conductance is site and season specific (significant positive relation only in the dry season and at the wet site). Crown conductance and its sensitivity to VPD exhibited consistent relationships with soil water content, the degree of anisohydry, and whole-tree hydraulic conductance. Future increases in VPD and drought will reduce crown conductance with large implications on water use and carbon uptake.

#### Future Climate Doubles the Risk of Hydraulic Failure in a Wet Tropical Forest

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Global changes drive conflicting responses in forest biomass, with rising carbon dioxide  $(CO_2)$  increasing productivity while rising vapor pressure deficit increases tree mortality. The net effect of these drivers is poorly understood, particularly in tropical forests. Hydraulic traits and water use strategies are critical in determining mortality risk under climate change. In this study, the team used a dynamic vegetation model with plant hydrodynamics (Functionally Assembled Terrestrial Ecosystem Simulator-Hydro) to simulate the response of gross primary productivity and hydraulic failure to future climate in a wet tropical forest. Researchers calibrated the model for Barro Colorado Island in Panama and selected plant trait ensemble members that performed well against observations. Selected members were run with temperature and precipitation anomalies from Coupled Model Intercomparison Project Phase 6 models for two greenhouse gas emission scenarios (SSP2-45 and SSP5-85) and two CO<sub>2</sub> levels (contemporary and anticipated). The simulations project productivity increases by 22% under SSP2-4.5 and by ~48% under SSP5-8.5. In simulations where CO<sub>2</sub> is held at contemporary levels, productivity decreases by ~25% under both scenarios in 2100. The risk of hydraulic failure increased from 4% to ~10% under each climate scenario, with or without elevated  $CO_2$ . The team further analyzed the variance in productivity, evapotranspiration, and hydraulic failure due to climate scenarios, CO<sub>2</sub>, and plant traits. Results suggest that rising mortality rates through hydraulic failure may offset increases in future productivity due to increasing CO<sub>2</sub> levels.

#### Disentangling the Effect of Humidity and Temperature in the Leaf Conductance Response to Vapor Deficit in Tropical Trees

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Understanding the response of stomata to changes in air temperature and humidity is key to predicting the future of tropical forests. Models that describe the behavior of stomata need to represent the response to rising temperature and drier air (a higher vapor pressure deficit) but differ in their approaches. The team examined the response of stomatal conductance to independent changes in temperature and relative humidity in five tropical tree species by manipulating leaf-level conditions using photosynthetic gas exchange analyzers. Researchers compared six formulations of steady-state conductance models that used different representations of photosynthesis and the evaporative demand on conductance. The team found that the best-fitting model used a nonlinear relationship between photosynthesis and stomatal conductance. Using relative humidity instead of vapor pressure deficit improved model performance when the temperature varied and resulted in similar performance when the humidity varied. The different stomatal conductance dynamics to changes in humidity and temperature showed that the underlying mechanisms associated with the stomatal response may be different. Moreover, the nonlinear relationship between photosynthetic rate and stomatal conductance suggests a sharper physiological response of tropical forests to extreme climatic conditions than previously acknowledged.

# Canopy to Root Zone Soil, Water, and Nutrient Dynamics from Field Observations Across Different Environmental Gradients in the Neotropics

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The ability to measure water and nutrient fluxes from the canopy to the root zone is key to understanding vegetation dynamics in tropical rainforests. Simultaneous measurements of these variables through time can provide powerful insights on the various processes responsible for changes in plant growth and function. The project pairs water volume and nutrient measurements from precipitation, throughfall, and subsurface soil water infiltration to investigate the dynamics of these fluxes across space and time. Sites were selected within tropical rainforests of Brazil, Panama, and Puerto Rico to investigate changes across different soil texture, seasonality, topography, and rainfall gradients. Each field site was conveniently co-located with additional observations that included temperature (air, plant, and soil), evapotranspiration, sap flow, soil moisture, soil matric potential, and leaf area index, which collectively aid in better constraining the impacts of these fluxes on plant function and growth as well as providing estimates of local water balance closure. Researchers compare the impacts of El Niño on these fluxes across sites given the difference in

proximity to the El Niño source region. In addition, subdaily infiltration observations were used to run an inverse model simulation within the HYDRUS-1D model to estimate the pedotransfer functions and the soil water retention curve (SWRC). Results reveal the importance of wet and dry season dynamics and soil texture on the water and nutrient fluxes as well as the importance of soil texture and topography in pedotransfer functions and the SWRC. This research will provide useful benchmarks of water and nutrient fluxes as well as soil properties within tropical rainforests that will be used in the development of the Functionally Assembled Terrestrial Ecosystem Simulator model.

#### Student

# Forest Dynamics After a Windthrow in the Central Amazon

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Windthrows are the most common natural disturbances in the Amazon causing changes in the dynamics and functioning of these ecosystems. Comprehensive data of the natural regeneration niches and species establishment represents a significant achievement in better understanding the susceptibility of disturbed areas to climate change. However, it is still unknown how these dynamics patches interact at the gap-phase regeneration. The team investigated the variations in the rates of recruitment and mortality every 2 months for 3 years in a gradient of disturbance severity and analyzed the factors that most affected these variations. The study site is located in an old-growth windthrown forest in Manaus, Brazil. The windthrow occurred in 2019. Inventory plots were installed in four classes of severity: high, medium, low, and undisturbed. Preliminary results showed a significant effect of disturbance severity and time post disturbance on recruitment rates (p<0.001), but no variations for mortality rates of saplings (p=0.3295). In the first year, in the high and medium severity classes, the recruitment was maximum and decreased until it was constant after the second year. In contrast, the mortality rates started to increase after the first year, presenting a peak in the second year of the study, but remain highly variable. Results demonstrate that even in 3 years the recruitment is highly dynamic across the severity gradient.

Changes in light availability caused by the windthrow increased the recruitment rates, but determining which characteristics are allowing the species succession still needs to be realized. The results of this research promoted a better understanding of how fast disturbances caused by the wind affect the functional composition and demographic rate of the forest.

#### Simulating Secondary Forest Growth and Composition Dependency on Prior Land Use, Time of Abandonment, and Seed Availability

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Land abandonment after agricultural use is a common phenomenon in tropical forest regions. Prior land use, time of abandonment, and seed availability influence secondary forest growth rates and trajectories of composition. Puerto Rico is an ideal setting to evaluate the ability to simulate secondary forest growth following land abandonment. Most of the island was under agricultural cultivation and subsequently abandoned over the course of the 20th century.

Island-wide estimates of forest age and current biomass allow for benchmarking E3SM Land Model-Functionally Assembled Terrestrial Ecosystem Simulator (ELM-FATES) simulations of secondary forest growth. The team has developed robust parameterizations for nine tropical plant functional types (PFTs), representing seven evergreen and two deciduous tree strategies. The evergreen PFTs are differentiated along axes of mature tree height, shade tolerance, and growth rates. The two deciduous PFTs are differentiated by mature tree height. These PFTs have been evaluated at a wet and dry site in Puerto Rico. Researchers created workflows to evaluate the relative importance of prior land use, time of abandonment, and seed availability within the current ELM-FATES infrastructure. Prior land use is evaluated by starting one set of simulations with established grass and another with a shade-tree coffee plantation. Seed availability is evaluated by manually editing the restart files to represent a dense and a sparse seed bank. Time since abandonment and the effects of the realized climate conditions will be evaluated by starting one set of simulations in 1936 and a second set in 1976 as those years correspond to the most common current forest age classes. All simulations are forced with 1-km climate data generated with the Daymet algorithm at

Oak Ridge National Laboratory. Results from these simulations allow the team to understand and prioritize model development tasks needed to effectively simulate secondary forest growth following agricultural land abandonment in the tropics.

# Linking Function and Life History Strategy to Soil Water Access in Panamanian Forests

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Soil water potential and effective root water sourcing depth are key factors that determine the availability of soil water to plants. Plant water uptake is further controlled by edaphic and environmental conditions and root, hydraulic, and stomatal characteristics that vary with plant-water use strategies. Understanding this variation is central to assessing vegetation responses to 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. Yet, such studies are limited in the humid tropics due to logistics and difficulty in timing water isotope sampling, which needs to occur during a significant dry-down period that allows evaporative isotopic separation of water within the soil profile. Furthermore, foundational studies conducted in the tropics have generally relied on only one isotope tracer, thereby limiting Bayesian and other mixing-model frameworks aimed at quantifying source water contributions. Here, the team reports findings on differential plant-water sourcing depths based on  $\delta^{18}O$ and  $\delta^2$ H, stem  $\delta^{13}$ C, and soil and plant water dynamics. These data were collected in 2022 from tree species with a range of ecological strategies and plant functional types at two forest sites in Panama: Parque Natural Metropolitano (PNM) and Barro Colorado Island, which include a range of growth-survival and stature-recruitment trade-off strategies. Data are being applied to test an inverse rooting model and results used to inform the Functionally Assembled Terrestrial Ecosystem Simulator (FATES), FATES-Hydro land models, and their simulations of tropical forest response to drought. In 2023 to 2024, there was a major El Niño-Southern Oscillation (ENSO) event that affected the neotropics, and additional samples were collected in PNM, the typically

wetter San Lorenzo site in Panama, and the ZF2 Research Forest in Brazil. Preliminary data from the ENSO will also be presented.

#### Diurnal Changes in Canopy Spectral Response to Drought Stress in an Amazon Forest

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Near-infrared (NIR) reflectance, particularly with Landsat imagery data, has been used in the central Amazon as a gauge for forest regrowth. As the frequency of severe droughts in the Amazon is expected to increase, coupled with droughts being found as a factor of increasing tree mortality, it is important to find indicators of drought impacts on tropical rainforests that can be applied at broader scales. Combining remote sensing tools with field data, the team is looking for links between NIR reflectance in these forests during times of extreme drought. In October 2023, researchers collected diurnal, multispectral imagery over the course of 2 weeks in a central Amazon Forest. This occurred during a period of extreme El Niño-Southern Oscillation-related drought. The team collected this data at multiple points throughout the day to evaluate diel patterns. Targeting individual trees attached with sap flow sensors, researchers also delineated the crowns of over 70 rainforest canopy trees, spanning a diverse wood density gradient. Combining remote sensing tools with individual-specific sap flow data, the project is looking to elucidate spectral patterns based on functional group responses as NIR reflectance while drought stress increases. The team will then evaluate if these crown patterns can be scaled up to be applied at a broader ecosystem level.

# Belowground Biogeochemistry Science Focus Area

### The Lawrence Berkeley National Laboratory Belowground Biogeochemistry Science Focus Area: Overview and Soil Carbon and Nitrogen Cycling

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In the Lawrence Berkeley National Laboratory Belowground Biogeochemistry science focus area (SFA), researchers study the role of soils in terrestrial biogeochemistry and future climate. The team aims to improve process-level understanding of ecosystem-climate interactions and to develop next-generation predictive capacity suitable for Earth system models. The research is centered around a set of field, laboratory, and model experiments to characterize how biotic and abiotic processes influence soil carbon and nitrogen (N) cycling. Applying experiments and models together is important for exploring how plant-soil-microbe interactions may shape ecosystem responses to a warming climate in the long term. Researchers are conducting two experiments. The Blodgett Forest whole-soil warming (+4°C) experiment was established in 2013. In 2020, the team doubled the number of experimental plots; heating these new plots started 7 years after the original warming experiment began, allowing researchers to investigate the effect of time explicitly. After 9 full years, heated plots still have carbon dioxide (CO<sub>2</sub>) respiration, with no detectable effect of warming duration. Future research will explore the relaxation response of microbial respiration and changes in tree belowground functional structure with warming. The Point Reyes grassland whole-soil warming experiment is in the pretreatment monitoring phase; heating will commence winter/spring 2024. In addition to providing a useful contrast to the conifer forest, the grassland experiment heats the whole root zone, allowing researchers to study coupled soil-microbe-plant warming responses, such as plant-soil N interactions and vegetation phenology and productivity. Researchers are also expanding the SFA's past focus on warming and soil carbon to encompass wildfire as a global change impact and driver, and vegetation dynamics in response. In this poster, the team will share recent highlights on the biogeochemical responses to warming (Task 1 of the

SFA). Research on microbiology (Task 2), geochemistry (Task 3) and wildfire (Task 5), and modeling (Task 4) are in posters by Karaoz, Crutchfield-Peters, and Riley respectively.

# The Role of Redox and Wildfire in Shaping the Fate of Soil Carbon and Biogeochemical Cycling

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Soils store more carbon globally than the biosphere and atmosphere combined, primarily as soil organic matter (SOM). The Belowground Biogeochemistry Science Focus Area (SFA) is tasked with using manipulation experiments to explore how soil carbon stocks will respond to a changing climate, and in particular to warming. Here researchers lay out two new areas of investigation for the SFA that will improve the understanding of the soil carbon cycle and how soil carbon stocks will respond to future climate conditions.

The majority of reactions that shape SOM decomposability involve electron transfer (or redox) reactions. These reactions are largely driven by microbial metabolisms, including aerobic and anaerobic respiration. However, redox status and dynamics in upland soils are understudied. Additionally, organic matter associations with redox-active minerals and metals also influence SOM decomposition, but the detailed behavior of those associations remains uncertain. To that end, researchers investigate dynamic redox conditions and SOM characteristics throughout the soil profile in a dynamically saturated coastal grassland in Northern California. Researchers report initial results from arrays of custom-made redox electrodes deployed in shallow, intermediate, and deep soil horizons alongside measurements of soil pore water and groundwater chemistry.

In parallel, researchers are launching a new investigation of soil biogeochemistry, including SOM cycling, and plant community recovery after wildfire. Here the team presents the design and initial testing of mobile warming units. These units will be deployed after fire in both a grassland ecosystem and mid-elevation forest during Phase 3 SFA. Once researchers establish baselines in temperature and moisture for control and warmed plots, they will investigate: 1) how SOM and metal cycling are affected by fire and warming, given the loss of vegetation, input of fire-derived mineral ash and pyrogenic carbon, and changes in soil moisture; and 2) how soil warming impacts the recovery of native and planted vegetation in fire-impacted ecosystems.

# Microbial Functional Traits Through the Whole Soil Profile and Their Response to Warming

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Subsoils contain the majority of global soil organic matter (SOM), whose depolymerization to dissolved organic carbon and mineralization to carbon dioxide  $(CO_2)$  is fundamentally microbially driven. An overarching goal of the Science Focus Area (SFA) is the development of mechanistic models that represent microbial metabolic, physiological and life history traits in a numerical model that accounts for interactions with plants, minerals, and environmental drivers, including temperature and moisture. Along the soil depth profile, the decreasing effects of plant inputs and rhizosphere interactions are major drivers of variation in SOM composition and transformation by microbes. This variation selects for microbiomes with distinct metabolic, physiological, and cellular traits that may constrain the trajectory and magnitude of the respiration response to warming through the soil profile.

To evaluate microbiomes and their trait distributions across the soil column under the effect of warming in the long-term field experiment at a conifer forest (Blodgett, CA), researchers utilized genome-centric metagenomics and furthermore assessed active metabolisms and SOM transformation pathways using metaproteomics and metabolomics. At the overall community level, soil depth, warming period, and warming treatment explained 41.5, 5.5, and 1.9% of the community variance, respectively, with multiple phyla represented in ~2,300 MAGs underlying these differences. Trait analysis of MAGs showed that denitrification, nitrite oxidation, degradation of complex carbohydrates, and one-carbon metabolism (for both methane and methanol) were prominent and phylogenetically widespread, with several genome representatives detected in the metaproteomes. Methanol and ethanol were highly abundant through the profile, whereas the abundance of more favorable substrates declined strongly. Transformations of alcohols and methyl compounds were among the most frequent potential transformations through the profile and increased with warming only in deeper soils. Together metagenomes,

metaproteomes, and metabolomes support a shift from metabolism of thermodynamically favorable plant-derived inputs (amino acids, sugars) to less favorable substrates with increasing depth.

# Microbe-Explicit Modeling Reveals Complex Interactions in a Forest Soil Heating Experiment

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Most soil heating experiments have found an increase in soil-surface carbon dioxide  $(CO_2)$  emissions  $(F_s)$  with heating, but inconsistent soil organic carbon (SOC) stock responses. To evaluate these patterns, researchers applied two microbe-explicit models, ELM-ReSOM and ecosys, to interpret heating impacts on a California forest ecosystem subjected to 1 m deep 4°C soil heating. Both models accurately simulated control-plot F<sub>st</sub> SOC stocks, root biomass, soil moisture and temperature, and the heating effect on  $F_s$ . Researchers applied uncoupled ELM-ReSOM to analyze direct soil heating effects. Researchers found large uncertainties associated with microbial temperature sensitivity, mineral adsorption capacity, and microbial and enzyme dynamics. Researchers analyze the modeled increase in total and component SOC stocks in topsoils and decreases in deeper soils. Researchers used the fully coupled ecosys model to explore a complex suite of interactions affecting the heating-induced increase in  $F_{s}$ , yet very small changes in SOC stocks. The modeled soil heating induced a cascade of effects: soil drying, reduced stomatal conductance, reduced NPP, reduced leaf and fine root allocation, reduced fine root biomass and exudation, and increased root litter inputs to soil. Soil heating led to about a 50% larger increase in root autotrophic respiration than in heterotrophic respiration, with the heating effect on both these fluxes decreasing over the simulation period. Increased heterotrophic respiration led to increased mineral nitrogen (N) availability and increased plant N uptake. Since most field studies are unable to make long-term observations of all these factors, researchers conclude that a coupled observational and mechanistic modeling framework is needed to interpret and explore the implications of soil heating experiments. These results highlight the challenges that microbe-explicit models face in accurately predicting the soil carbon cycle response to future warming across space and time.

# Soil Carbon Dynamics Science Focus Area

# Ground Ice Variations Among Soil Horizons and Ice-Wedge Polygon Types in Arctic Coastal Lowland Soils

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In Arctic coastal lowlands dominated by ice-wedge polygons (IWPs), a better understanding of near-surface ground ice quantities and their spatial distribution is needed to improve model predictions of ecosystem and landscape responses to climatic change. In investigations of how IWP geomorphology (trough vs. center), size, and types (i.e., flat-, low-, and high-centered IWPs) affect the distribution and composition of soil organic carbon (SOC) stocks, the team also collected considerable ground ice data. These data estimate the spatial distribution of volumetric ice contents to depths of up to 3 meters within the cross-section stratigraphy of soil horizons and ice wedges for transects running from trough center to trough center of sampled IWPs. Data from nine IWPs (three of each type) located in the thaw-lake terrain near Utqiagvik, AK, indicate that the greatest volumetric ice contents occurred, on average, at depths between 0.45 m and 1 m in the upper permafrost of high-centered IWPs, due mostly to proportionately larger areas occupied by the ice wedges. Averaged across all IWP types, organic and mixed organic/mineral horizons generally had greater volumetric ice contents than mineral horizons. Not surprisingly, the team found a strong negative relationship between ice content and soil bulk density due to the frequent occurrence of excess ice. However, the team also observed a positive relationship between ice content and SOC density (kg C  $m^{-3}$ ). Future work will compare the ground ice contents observed near Utqiagvik and their relationships with IWP type, soil horizon type, and SOC density to that of polygonal landscapes formed on other soil parent materials.

#### Soils of the Arctic Foothills of Alaska: Composition and Degradation State

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The Arctic Foothills of Alaska are characterized by rounded hills and plateaus with continuous permafrost soils covered in tundra vegetation. The region undergoes permafrostaffected processes, such as solifluction and other lateral mass movements, cryoturbation, and patterned-ground formation, impacting soil organic matter (SOM) accumulation, composition, and degradation. Anthropogenic activities and climate change have intensified press and pulse thaw disturbances, potentially leading to downstream soil movement and exposure of SOM that has been cold-stabilized for thousands of years. However, information is limited on the composition of the SOM that might be mobilized by these processes. Here, researchers investigated the composition and degradation state of SOM across landscape positions in the Arctic Foothills.

Two toposequences, formed on land surfaces of differing ages, were examined, encompassing seven hillslope positions: summit, shoulder, upper- and lower-back slopes, upper- and lower-foot slopes, and basin. Researchers used mid-infrared spectroscopy to examine variations in organic functional groups and minerals across soil horizon types and slope positions. The ratio of aromatics to polysaccharides was calculated as an indicator of SOM degradation state. Researchers identified 14 influential wavelength bands across toposequences, horizons, and slope positions. The abundance of organic functional groups, associated with phenolic OH, aliphatics, and polysaccharides were lowest in mineral horizons and varied between organic and mixed organic-mineral horizons. These organic groups also differed between toposequences and across slope positions. Conversely, bands characteristic of amides and aromatics were consistent across toposequences, horizons, or slope positions. Spectral bands indicating clays varied across toposequences and slope positions but not among horizon types, whereas general silicate bands were more pronounced in mineral horizons. The ratio of aromatics to polysaccharides indicated consistently more degraded SOM occurred in mineral horizons. In summary, slope position significantly influenced SOM composition (particularly phenolics,

aliphatics, and polysaccharides) and clay content, with mineral horizons containing more degraded SOM.

# Terrestrial Ecosystem Science Science Focus Area

# Plant Community Changes in Annual Production and Composition Through 8 Years of Warming Manipulations Under Ambient and Elevated Carbon Dioxide Atmospheres

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The Spruce and Peatland Response Under Changing Environments (SPRUCE) experiment has operated five warming manipulations (+0, +2.25, +4.5, +6.75, and +9°C) with and without elevated carbon dioxide atmospheres (eCO<sub>2</sub> of +500 ppm) for 8 full calendar years (since August 2015). Researchers have tracked shrub-layer vegetation responses to the treatments using annual destructive plot sampling within each of the experimental plots. In 2023, the team sampled three 0.4 m<sup>2</sup> plots from three random locations with each of the treatment enclosures (plus two ambient plots) to evaluate the influence of the warming and eCO<sub>2</sub> treatments on community composition, standing biomass, and annual above ground net primary production (ANPP). Plot-level cumulative stand biomass has increased with warming treatments. Pretreatment and colder plots have standing mass in the range from 147 to 300 gC m<sup>-2</sup> with warmer treatment plots ranging from 462 to 640 gC m<sup>-2</sup>. The 2023 assessment shows standing biomass combined across species for the +4.5, +6.75, and +9°C warming treatments with a trend of higher biomass under eCO<sub>2</sub>. Within the mid-summer standing biomass pool woody tissues drive the difference with foliage being very similar across all experimental treatments. ANPP is quite constant across treatments for the 2023 assessment ranging from 60 to 150 gC m<sup>-2</sup> y<sup>-1</sup>.

The plant community composition was assessed for key ericaceous shrubs (*Rhododendron, Chamaedaphne, Kalmia*), two *Vaccinium* species (*V. angustifolium, V. oxycoccos*), graminoid species (mostly *Eriophorum*) and one common forb *Maianthemum trifolium*, plus a few minor understory

and two tree species (*Picea, Larix*). The composition has changed with 8 years of treatments. Under all warmed scenarios >+4.5°C *Kalmia, V. oxycoccos,* and *M. trifolium* are largely absent from the plots. *Rhododendron* and *Chamaedaphne* have maintained their presence in the community and *V. angustifolium* plants and *Picea rubrum* seedling are showing increases.

# A Framework for Evaluating Process Uncertainty Among Soil Carbon Models

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Microbial and mineral interactions mediate soil carbon (C) responses to environmental change. These interactions are numerous and often result in complicated or counterintuitive soil responses. The newest generation of soil C models attempt to predict these responses by explicitly representing some microbial and mineral processes. However, these models make vastly different predictions. This model uncertainty is driven largely by process-knowledge uncertainty. That is, different models represent different combinations of hypotheses about the processes governing soil C dynamics. Reducing this process uncertainty and homing in on optimal process representation in soil C models requires: (1) identification of key processes that drive divergence among models; and (2) empirical efforts targeted toward a better understanding of these hypotheses. Here, researchers discuss the progress on developing and applying a multi-assumption soil C model within the multi-assumption architecture and testbed (MAAT) to evaluate the factors that underlie uncertainty among several microbially explicit soil C models. MAAT is a modular modeling code that can easily vary model process representations, with built in tools for model calibration and process- and parameter-level sensitivity analyses. Researchers have implemented several soil C models in MAAT and found that these models simulate markedly different responses of soil carbon to alterations in inputs, temperature, and moisture. Alternative hypotheses about mineral-associated C turnover and microbial biomass dynamics account for a large portion of this uncertainty in response to altered soil C inputs. Researchers will discuss progress in calibrating models against a common dataset to control for differences in model parameterization that

can confound the comparison of process representation among models.

Future work will focus on implementing nutrients into the multi-assumption soil C model and combining model development and optimization with forthcoming experimental incubations and field datasets.

#### Effect of Warming on Solute Concentrations and Fluxes from Peatland Streams

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Increased temperatures are altering biogeochemical processes in peatlands. Because many peatlands are hydrologically connected to downstream ecosystems, biogeochemical alterations within peatlands may also affect these connected environments. In the Spruce and Peatland Under Changing Environments (SPRUCE) experiment, the team is examining how warming affects solute concentrations and fluxes from peatland streams. At SPRUCE, each experimental enclosure is surrounded by a belowground corral, which hydrologically isolates each plot. Two lateral, slightly sloped, slotted pipes in the near-surface peat allow for lateral, passive drainage of water out of each enclosure, akin to stream flow.

Stream water drains into a subsurface basin, which is equipped with a water-level sensor to estimate stream flow and an automated sampler to collect flow-weighted water samples. Water samples are retrieved weekly and analyzed for total organic carbon (TOC), inorganic and total nutrients, anions, cations, and metals. After 7 years of warming, researchers have observed many changes in stream water solute concentrations. Notably, TOC concentrations have increased with warming, from 52 mg/L (+0°C enclosures) to 87 mg/L (+9°C enclosures). Concentrations of cations and metals (i.e., calcium, magnesium, aluminum, iron), several of which form complexes with TOC, have also increased with warming. While these increases in solutes may reflect evaporative concentration, there was a muted response of chloride concentrations (a conservative ion) to warming. Therefore, increased TOC, cation, and metal concentrations likely reflect warming-induced increases in peat mineralization, rather than a solely physical (evaporative concentration) response. While concentrations of many solutes have increased with warming, stream flow has decreased, likely due to increased evapotranspiration, resulting in an overall decrease in solute efflux from the peatland. In summary, climate change may alter the chemistry and volume of stream

water flowing from peatlands, with potential cascading effects to downstream ecosystems.

#### Tracking Down the "Missing Energy" at Eddy Covariance Sites: Have Researchers Been Miscalculating Sensible Heat?

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The surface energy imbalance problem has plagued the eddy covariance community (EC) for decades. Essentially, when researchers add up all the measured heat fluxes and energy storages, balance is not achieved, and there is a significant non-zero residual that reflects a systematic underestimation of around 20%, which can be 100 W m<sup>-2</sup> or more—hence the notional "missing energy". The lack of closure calls into question the accuracy of the EC technique and/or knowledge of the micrometeorological system. Regardless of which is true, there are broad implications for downstream users of EC data. Eddy covariance data is widely used for validating Earth system and remote sensing models, and increasingly in applications that intersect with regulatory and legal spheres. Solving the EC energy imbalance problem is thus of prime importance to numerous scientific disciplines, and broader society. Despite many years of work, the EC community has not reached a consensus on the causes and remedies needed to solve the surface energy imbalance problem. Here, the team reexamines the surface energy imbalance problem through the lens of first principles of physical fluid mechanics and thermodynamics, hypothesizing that researchers have been using the wrong theory and equations for computing the sensible heat flux (H). Typically, *H* is determined from the eddy covariance between w and T (w and T are the vertical wind velocity and air temperature, respectively). The heat transport associated with the mean motion of air and several other terms are deemed small and unimportant, mainly due to the use of a "base temperature", "from which each element of air is warmed (or cooled) during the vertical transfer of heat supplied (or removed) at the underlying surface" and from which actual air temperature is only several degrees different at most. Here the team shows that this theory is fundamentally flawed. Researchers will derive the net ecosystem sensible heat exchange from the fundamental equations of fluid mechanics and thermodynamics. Here, the team will present the new equation set and preliminary test results.

# Improving Simulations of Carbon Cycle Feedbacks Through Integration of ELM with Observations and Experiments in Vulnerable Ecosystems

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Carbon cycle feedback parameters estimated by the current generation of Earth system models may be underestimated due to missing processes and uncertain parameters. One key shortcoming is that most land-surface models do not represent peatlands, which cover a relatively small fraction of Earth's surface but contain a much larger proportion of terrestrial carbon stocks that may be vulnerable to environmental change. The Spruce and Peatland Responses Under Changing Environments (SPRUCE) whole-ecosystem warming and elevated carbon dioxide  $(CO_2)$  experiment began in 2015 in an ombrotrophic bog in Northern Minnesota and will continue through 2025. Results to date indicate strong releases of carbon (C) from warming. This results from a combination of factors including increased heterotrophic respiration, increased methane  $(CH_{4})$  emissions, and a loss of productivity and coverage of Sphagnum mosses. Upscaling SPRUCE to better understand regionalscale feedbacks requires a process-based modeling approach. In addition to missing peatland and wetland processes, many parameters regulating C feedbacks in surrounding upland systems are also uncertain. The most vulnerable C stores of boreal and temperate ecosystems may be those in vegetation or organic soils located near ecological boundaries, including at SPRUCE, which is at the southern edge of the boreal zone. Researchers introduce a new version of the Energy Exascale Earth System Model (E3SM) land component that is augmented to include peatland processes (ELM-Peatlands), which is initially tuned using SPRUCE observations and scaled regionally using a combination of remote sensing and ground-based observations. Researchers use a neural network-based surrogate modeling approach to constrain ELM parameters for five major plant functional types using observed carbon and energy fluxes from long-record AmeriFlux wetland and forested upland sites. Researchers present initial simulations using the constrained ELM-Peatlands over a regional domain covering central North America and compare feedback parameters estimated in this model to those in the CMIP6 ensemble.

#### Nitrogen and Phosphorus Pools and Turnover in Peat Following 5 Years of Simulated Climate Change

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Boreal peatlands currently store large amounts of carbon (C) and will be exposed to higher temperatures and elevated levels of atmospheric carbon dioxide  $(eCO_2)$  in the coming decades. The Spruce and Peatland Under Changing Environments (SPRUCE) experimental site in northern Minnesota is a forested, ombrotrophic bog that has been subjected to experimental warming and eCO<sub>2</sub> treatments since 2016. In 2021, the team sampled the top 30 cm of the peat at SPRUCE and began a year-long laboratory incubation to assess pool sizes and turnover of C, nitrogen (N) and phosphorous (P) in the rhizosphere. Mineralization of C, N, and P was quantified by measuring carbon dioxide  $(CO_2)$ ,  $N_2O_2$ , and methane (CH<sub>4</sub>) gas fluxes as well as NH<sub>4</sub>, NO<sub>3</sub>, and PO<sub>4</sub> in soil leachate. The optimized decomposition conditions and extended timeframe of the laboratory incubation meant that total mineralization cumulative mineralization curves fit with exponential decay models could be explored for the three elements. Preliminary results from this experiment indicate that 5 years of experimental field manipulations have significantly impacted pool sizes and cumulative mineralization of these critical elements in the rhizosphere. Total CO<sub>2</sub> mineralized significantly decreased with field temperature and, in surface soils, slower CO<sub>2</sub> mineralization was explained by a higher proportion of soil C being present in an inactive versus active cycling C pool. The bulk %N of incubated peat increased broadly with depth (p=0.09) but notably increased with field temperature (p=0.01). Total NH4 mineralization significantly increased with field temperature and this increase was greater than expected based on the higher bulk soil %N alone. Total PO<sub>4</sub> mineralization was not impacted by the experimental treatments. These findings indicate that C, N, and P cycling in warmed rhizosphere at SPRUCE has become uncoupled during the first 5 years of experimental warming due to actively cycling C being lost and peat N being found in more readily mineralized forms.

# Microbial Community Dynamics During 3 Years of *In Situ* Peat Decomposition at the SPRUCE Experiment in Northern Minnesota

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Peatlands ecosystems act as major global carbon sinks, as primary production outpaces organic matter decomposition resulting in massive soil carbon deposits that account for greater than one third of all soil carbon. Prior investigations as part of the Spruce and Peatland Response Under Changing Environments (SPRUCE) experiment have shown that warming treatments are altering peatland biogeochemistry, greatly increasing the efflux rates of both carbon dioxide  $(CO_2)$  and methane  $(CH_4)$  from the ecosystem manipulation chambers. In order to better understand microbial dynamics contributing to these changes, the team deployed a series of depth specific decomposition bags attached to rigid frames (e.g., peat ladders) in triplicate across the temperature and CO<sub>2</sub> treatment enclosures for 3 years. At harvest the team characterized Bacteria, Archaea, and Fungi community dynamics through amplicon sequencing and measured peat mass and peat chemistry changes. These results showed that microbial communities were significantly affected across soil depths, temperature and temperature x CO<sub>2</sub> treatments in the experiment and that diversity increased with temperature treatments. Microbial communities also showed greater degrees of complexity and across network analyses and an increase in highly connected hub taxa with increasing temperatures that included methanogens. Despite this, peat soil decomposition showed no significant effects on soil mass loss or chemical composition after 3 years in situ incubation, with only ~4.5% mass loss overall. These results are planned to be revisited from additional peat ladders that were deployed at the same time as researchers wrap up the final years of the SPRUCE experiment. This and previous studies from the SPRUCE experiment have now shown that warming is accelerating microbial community change, organic-matter decomposition, and subsequently CO<sub>2</sub> and CH<sub>4</sub> production from these globally important carbon reservoirs, raising the overall level of concern for climate change driven positive feedback loops from these ecosystems.

#### Peatland Greenhouse Gas Efflux (CO<sub>2</sub>, CH<sub>4</sub>) Increases Due to Plant-Microbial Dynamics in Response to Whole Ecosystem Warming

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Peatlands, although only covering a small portion of the land surface store around one third of soil carbon. This high amount of carbon sequestration is sustained by climate; hydrology and temperature trends sustain high water tables that promote autotrophic carbon fixation and prevent aerobic decomposition. These carbon stores are tied to complex ecosystem processes such as plant and microbial community composition and may be threatened by future warming. To test the sensitivity of these carbon stocks to climate change scenarios researchers utilize the whole ecosystem manipulation of the Spruce and Peatland Under Changing Environments (SPRUCE) experiment in northern Minnesota.

Here researchers present greenhouse gas flux (GHG: carbon dioxide-CO<sub>2</sub> and methane-CH<sub>4</sub>) across experimentally warmed (from +0 to +9°C) and elevated atmospheric CO<sub>2</sub> (+500 ppm). Researchers use automated clear-top gas flux chambers to measure changes in net ecosystem exchange (NEE) CO<sub>2</sub> and CH<sub>4</sub> four times per hour during the growing season of 2022 and 2023. Researchers compare gas flux measurements to a suite of other environmental response variables: photosynthetically active radiation, water table depth, and soil temperature and moisture.

These results show: GHG flux increases with warming soil temperatures, net carbon flux to the atmosphere increases following a linear relationship. Water table depth and temperature preconditions dynamics may cause switch between the dominant gas flux between  $CO_2$  and  $CH_4$ .

In addition, measured CO<sub>2</sub> NEE showed that elevated CO<sub>2</sub> plots had increased daytime uptake of CO<sub>2</sub> during the growing season, possibly due to CO<sub>2</sub> fertilization effects. However, this increased uptake was outweighed by increased ecosystem respiration. Furthermore, CH<sub>4</sub> flux was more dominant in ambient CO<sub>2</sub> levels, indicating complex ecosystem feedback effects.

Future work will be focused on key peatland carbon relationships such as;  $CO_2$  fertilization changes to water table and microbial community dynamics, increased individual plant function and plant functional type transitions within experimental plots.

# Greater Shrub Root Production Under Warming and Elevated Carbon Dioxide Is Not Distributed More Deeply

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Peatlands store a disproportionate amount of terrestrial soil carbon (C) relative to their global spatial extent (roughly 44% vs. 3%). The accumulation and stability of this C is impacted by the amount, timing, and depth distribution of plant root production. These aspects of plant root growth are in part determined by plant functional type (PFT), which are likely to be differentially sensitive to increased atmospheric carbon dioxide  $(CO_2)$  and temperatures. Common vascular PFTs in boreal bogs are: coniferous trees and ericaceous shrubs with shallowly and non-woody sedges plus forbs with deeply, distributed roots. The team estimated the effects of elevated CO<sub>2</sub> and whole-ecosystem warming (WEW) on root production in the Spruce and Peatland Response Under Changing Environments (SPRUCE) experiment in an ombrotrophic boreal bog in northern Minnesota, U.S. To date shrub productivity has increased dramatically in response to warming, both aboveground and belowground. The team hypothesized this response was due to: (1) shrub rooting depth tracking depressed water tables; and (2) longer growing seasons for shrub roots. WEW treatments ranged from 0 to +9 °C, in 2.25 °C steps above ambient temperatures.

These WEW treatments are crossed by ambient and elevated (+500 ppm)  $[CO_2]$  (*n*=10). Root production, timing and depth distribution were estimated from minirhizotron images collected throughout the year from 2015 to 2021. Shrub root production increased with WEW, and this response was stronger with elevated CO<sub>2</sub>. Growing season length for shrub roots did not respond consistently to WEW nor elevated CO<sub>2</sub>. Rather, on average, shrubs with +6.75°C WEW (both ambient and elevated CO<sub>2</sub>) grew their roots later in the year (c. Oct. 1) compared to all other plots (c. Aug. 7). Shrub roots grew more shallowly, rather than more deeply, with WEW. Researchers attribute this response in part to the lack of water table depression with WEW, but also to the distribution of nutrients.

#### Ecosystems Under Stress: Knowledge Gaps and Approaches Using MOFLUX as a Testbed

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Drought and heat are important stressors that influence forest ecosystem processes and biosphere-atmosphere gas exchange. The Missouri Ozark AmeriFlux (MOFLUX) site, situated in the central U.S. forest-grassland transitional zone, experiences frequent droughts and heat stress episodes. Indeed, drought plays a key role in shaping temporal variations of gas exchange within and across years, as well as stand composition through pulses of drought-induced tree mortality. Here, researchers synthesize new research aimed at broadly answering the question: how does drought and/ or heat stress influence the spatiotemporal variations of the forest carbon cycle? Specific questions include: (1) How does drought and temperature influence the spatial variation of soil respiration? (2) How do drought and heat stress influence the surface energy imbalance?; and (3) How does heat stress influence isoprene production and atmospheric chemistry? To address these questions, the team leveraged the long-term data record that was started in 2004, as well as opportunistic volatile organic compound (VOC) measurements made during the 2023 growing season using proton transfer reaction-time of flight-mass spectrometry (PTR-TOF-MS). VOC emissions are important plant stress responses and are associated with the protection of sensitive plant tissues when energy supply overwhelms energy demand during drought and heatwaves. Answering these intersecting questions will help guide future monitoring efforts to ensure that spatiotemporal variations are adequately characterized and enhance integrated scientific understanding of how temperate broadleaf forests dynamically respond to drought and heat stress.

#### Disentangling the Impacts of Warming and Drying on Peatland Ecosystems

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#### https://mnspruce.ornl.gov

Peatland ecosystems play significant roles in the global carbon cycle. Although only covering 2 to 3% of land's surface, peatland ecosystems store about one third of global soil carbon (C).

Warming in northern peatland may accelerate the soil carbon decomposition and lead to rapid release of carbon dioxide  $(CO_2)$  into the atmosphere, driving a positive land carbon-climate feedback. In addition to the direct impacts of warming on plant physiology, ecosystem respiration and community composition, warming could lead to the drop in the water table, which could also have important consequences for peat decomposition, community composition and ecosystem functions. The objective of this study is to disentangle the impacts of warming and drying on peatland ecosystems using a modeling approach at the Spruce and Peatland Responses Under Changing Environments (SPRUCE) site. Specifically, researchers use ELM-SPRUCE, a version of the E3SM (Energy Exascale Earth System Model) land surface component (ELM) for peatlands, to address the following questions: (1) Is ELM-SPRUCE able to capture warming responses under ambient CO<sub>2</sub>?; and (2) How much of C loss at SPRUCE is due to direct warming? How much of C loss at SPRUCE is due to changes in water table associated with warming? How much of C loss at SPRUCE is due to loss of sphagnum cover?

### AmeriFlux

#### AmeriFlux Management Project: Overview and the Year of Remote Sensing

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#### https://ameriflux.lbl.gov

AmeriFlux is a network of sites and scientists measuring ecosystem carbon, water, and energy fluxes across the Americas using eddy covariance techniques and the many scientists who use these data. The DOE-funded AmeriFlux Management Project (AMP) aims to enhance the value of AmeriFlux for Earth system modeling, terrestrial ecosystem ecology, remote sensing, and many other fields. To do this, AMP has teams focused on four tasks: (1) technical support and quality assessment/quality control (QA/QC), (2) data support and QA/QC, (3) core site support, and (4) outreach. The network continues to grow. In January 2024, AmeriFlux registered its 641st site. The team makes 3,360 site years of flux/met data from 478 sites publicly accessible. These data are used by a large community of scientists and practitioners worldwide. To maintain a high level of support, AMP invests in new data services and is pioneering a new mode of evaluating each site's data quality (e.g., remote data "visits" and mini workshops). The project also benefits from productive partnerships. For example, the National Ecological Observatory Network's 47 AmeriFlux sites make it the single largest network-within-the-network. Researchers co-develop data standards and products with the Integrated Carbon Observation System Ecosystem Thematic Centre. The team collaborates with the National Science Foundation-funded FLUXNET-Coop, which co-sponsors workshops, builds early career resources, and strengthens international connections among flux networks. This poster will highlight some of these recent activities, ongoing initiatives for remote sensing and urban fluxes, and special offerings for scientists regardless of previous level of experience, such as the Rapid Response Systems (loaner eddy flux systems for urban environments and other research opportunities) and systems available for DOE Atmospheric Radiation Measurement campaigns (e.g., in the Southeast United States). See also Housen Chu's AMP poster on a new data paper and the AmeriFlux FLUXNET data product. Come by the poster or write to AMP to share how AMP and terrestrial flux data can enhance further work.

# AmeriFlux BASE Data Pipeline to Support Network Growth and Data Sharing

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https://ameriflux.lbl.gov

AmeriFlux is a network of independent research sites that measure carbon, water, energy, and momentum fluxes between ecosystems and the atmosphere using the eddy covariance technique to study a variety of Earth science questions. AmeriFlux's diversity of ecosystems, instruments, and data processing routines all create challenges for data standardization, quality assurance, and sharing across the network. To address these challenges, the AmeriFlux Management Project (AMP) designed and implemented the BASE data processing pipeline. The pipeline begins with data uploaded by the site teams, followed by the AMP team's quality assurance and quality control (QA/QC), ingestion of site metadata, and publication of the BASE data product. The pipeline automated and facilitated communication, tracking, QA/QC, and publication functions, enabling the team to keep pace with the rapid growth of the network. As of January 2024, the AmeriFlux BASE data product contained 3,360 site years of data from 478 sites with standardized units and variable names of more than 60 common variables, representing the largest long-term data repository for flux-met data in the world. AMP further applied the Open Network-Enabled Flux processing codes to generate the FLUXNET data product for AmeriFlux sites. The FLUXNET product contains footprint-aggregated data that have been gap-filled, partitioned, and corrected for energy balance closure and includes uncertainty analysis. As of January 2024, the FLUXNET data product contained 1,381 site years of data from 195 sites.

# **FACE-Model Data Synthesis**

# Simulating CO<sub>2</sub> Responses of Secondary-Succession Forests at Duke and Oak Ridge FACE Experiments with ELM-FATES-CNP

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https://www.ornl.gov/content/free-air-carbon-dioxideenrichment-face-datamanagement-system

Rising atmospheric carbon dioxide  $(CO_2)$  can increase vegetation biomass production, which at the global scale can slow atmospheric CO<sub>2</sub> growth rates. Elevated atmospheric CO<sub>2</sub> (eCO<sub>2</sub>) experiments have demonstrated significant gains in net primary productivity (NPP) and biomass. Many terrestrial biosphere models have also indicated that eCO<sub>2</sub> has caused a large fraction of land carbon sequestration during recent decades and predict that this sequestration will continue to increase into the future. Another significant component of global change has been the conversion of primary forests to secondary forests and several ecosystemscale Free Air Carbon Dioxide Enrichment (FACE) experiment were sited in plantations. Analysis of these FACE experiments indicated that the variability in the  $eCO_2$ response is related to the stage of stand development and progressive nitrogen limitation. Researchers use the E3SM Functionally Assembled Terrestrial Ecosystem Simulator (ELM-FATES-CNP), a size and time-since-disturbance structured vegetation demography model that integrates carbon and nutrient cycling to investigate nutrient constraints on eCO<sub>2</sub> responses in even-aged forests. The primary objective of this study is to evaluate the performance of the ELM-FATES-CNP model against the observations from Duke and ORNL FACE experiments to ascertain how best to apply ELMFATES-CNP to investigate stand structure and nutrient controls on ecosystem carbon responses to eCO<sub>2</sub>. Understanding the interactions of nitrogen availability for plant uptake and growth is necessary to improve predictive capabilities of models to simulate ecosystem carbon storage in response to  $eCO_2$ . The team compared the net primary productivity (NPP) responses under simulated post-disturbance and counter-factual "equilibrium" forests at Duke and Oak Ridge. Researchers also use a carbon-only version of the model alongside two soil nutrient cycling hypotheses to evaluate the strength of nutrient limitation in FATES-CNP.

# Terrestrial Ecology DOE Early Career Projects

#### Soil Production and Chemical Weathering Rates from Intrusive Bedrock in the East River in Colorado

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The productivity of aquatic and terrestrial ecosystems relies on the release of essential elements from bedrock. The rate at which elements become accessible to biota depends on the rate soil is produced from bedrock by both physical and chemical weathering. Steep mountain catchments are global hot spots for erosion and weathering and hence strongly influence global biogeochemical cycles. However, there are still outstanding questions regarding the mechanisms of soil production and solute generation in mountain landscapes. Here, the project investigates the role vegetation plays in influencing soil production and chemical weathering within the East River watershed in Colorado. The team collected soils from forest (n=5) and alpine (n=4) ecosystems on intrusive igneous rocks and used cosmogenic nuclides and geochemical mass balance to determine soil production and chemical weathering rates. The mean chemical depletion fractions for forest and alpine soils were 0.27 and 0.15 respectively, indicating chemical weathering is a much higher proportion of soil production in forest versus alpine sites. Beryllium-10 concentration measurements are pending for additional samples, but preliminary results from forest (n=1) and alpine (n=3)indicate soil production rates are approximately 0.05 millimeter per year and 0.03 mm yr<sup>-1</sup>, respectively, suggesting bedrock is more rapidly converted to soil in the forest. Soil chemical weathering rates are 0.013 mm yr<sup>-1</sup> and 0.006 mm yr<sup>-1</sup> in the forest versus alpine sites, indicating that solute production in forests is higher than alpine sites. These findings suggest that migration of forests to higher elevation as climate changes will be accompanied by increases in solute generation and fundamental changes to alpine soils.

#### Tropical Forest Response to a Drier Future: Measurements, Synthesis, and Modeling of Soil Carbon Stocks and Age

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Tropical forests account for over 50% of the global terrestrial carbon sink and 29% of global soil carbon, but the stability of carbon in these ecosystems under a changing climate is unknown. Recent work suggests moisture may be more important than temperature in driving soil carbon storage and emissions in the tropics. However, data on belowground carbon cycling in the tropics is sparse, and the role of moisture on soil carbon dynamics is underrepresented in current land surface models, limiting the ability to extrapolate from field experiments to the entire region. The team measured or attained data for soil carbon stocks and radiocarbon  $({}^{14}C)$ values of profiles from over 40 sites spanning 12 pantropical regions. Project sites represent a large range of moisture, spanning 710 to 4,200 millimeters of mean annual precipitation (MAP), and include Alfisols, Andisols, Inceptisols, Oxisols, and Ultisols. Researchers found a large range in soil <sup>14</sup>C profiles between sites, and in some locations, the team also found a large spatial variation within a site. MAP explains some of the variation in soil <sup>14</sup>C profiles and carbon stocks, with smaller carbon stocks and younger soil carbon in drier forests. However, differences in soil type contribute substantially to observed variation across the dataset and with constrained gradients in moisture and parent materials in Panama. The project compares measured soil profile <sup>14</sup>C and carbon stock values to those modeled with the E3SM Land Model version 1 to demonstrate the utility of soil carbon and <sup>14</sup>C for benchmarking.

# Watershed Sciences

Watershed sciences research supported by the Environmental System Science program seeks to advance a robust, predictive understanding of how watersheds function as integrated hydro-biogeochemical systems, as well as how these systems respond to disturbances such as changes in water recharge, availability, and quantity; contaminant release and transport; nutrient loading; land use; and vegetative cover.

# Watershed Sciences University Projects

# Anaerobic Methane-Oxidizing Microbiomes in Agriculturally Influenced Riparian Zones and Their Linkage to Reactive Nitrogen Removal

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Anaerobic methane oxidation (AMO) is a microbemediated process active in anoxic aquatic habitats. Riparian zones (RZs) along streams in agricultural regions may be hot spots for anaerobic cycling of methane and inorganic nitrogen from leaching of excess fertilizer. However, AMO in RZs, and its potential linkage to nitrogen cycling, remains largely uncharacterized. Agricultural lowlands in the Judith River Watershed (JRW) of central Montana harbor aquifers with elevated reactive nitrogen loading and riparian aquifers that consistently display biogeochemical signatures associated with denitrification. Microbiome exploration of these riparian aquifers has suggested relatively high abundances of 16S rRNA genes related to Candidatus methylomirabilis, a bacterium known to link methane to nitrogen cycling through nitrite-dependent anaerobic methane oxidation (N-DAMO). Metabolic activity from this species would suggest a role for N-DAMO in both methane and nitrogen removal from the JRW with implications on models of greenhouse gas emissions. Goals of the project include: (1) characterize methane and other redox-sensitive compounds in JRW-RZ porewater under contrasting hydrological conditions; (2) identify genes and transcripts associated with N-DAMO and other relevant biogeochemical processes; (3) quantify AMO activity over relevant oxygen concentrations; and (4) adapt thermodynamically constrained

biogeochemical models of microbial metabolisms to predict the scale of N-DAMO (and other AMO processes) in RZs.

Metagenomic analyses have extended the evidence for N-DAMO as the dominant AMO process based on the recovery of particulate methane monooxygenase (*pmoA*) genes matching *Ca.* methylomirabilis. Genes diagnostic for canonical denitrification were also recovered at high frequency, while genes of anaerobic ammonium oxidation (anammox) were present but less common. These results indicate a complex anaerobic community with diverse pathways of both AMO and nitrogen loss. Incubation experiments will quantify rates of these processes over environmental gradients, informing development of RZ biogeochemical models that properly account for the influence of AMO.

# Deciphering the Role of Anaerobic Microsites for Hot Spot and Hot Moment Dynamics of Metal Redox Chemistry and Methane Emissions Within Riverine Floodplains

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Rates and reactions of biogeochemical (BGC) processes vary in space and time to produce hot spots and hot moments of elemental cycling. These dynamics are particularly enhanced at terrestrial-aquatic interfaces (TAIs), such as floodplains with strong redox fluctuations. Anaerobic microsites are zones of oxygen depletion in otherwise oxic soil environments, which can serve as redox hot spots, generating and exporting anaerobic BGC products, such as methane ( $CH_4$ ). Despite the importance of anaerobic microsites in TAIs, significant knowledge gaps still exist regarding their abundance, spatial distribution, and specific contributions to BGC processes, especially  $CH_4$  production. Hence, there is limited data to support model parameterizations and predictions of the impacts of anaerobic microsites on BGC functions at the field scale.

The main objectives of this study are: (1) to quantify the abundance and the impact of anaerobic microsites on methanogenesis and link this to elemental speciation and abundance of trace metals of importance for methane-cycling; (2) to compare microscale anaerobic microsite characteristics with macroscale observations on the field scale for methane emissions; and (3) to quantify reaction kinetics of relevant BGC processes within anaerobic microsites.

The Laboratory for Observing Anaerobic Microsites in Soils (LOAMS) is a novel approach that utilizes the fact that X-ray fluorescence 2D mapping can reliably detect, quantify, and characterize anaerobic microsites in natural soil core slices (up to 100 cm long) at µm-scale resolutions. To date, LOAMS investigations have revealed direct evidence of iron (Fe) and sulfur (S) reducing microsites in predominantly oxic toeslope soils (Pumphouse Lower Montane site by East River, CO), where anaerobicity would typically not be expected. In parallel, the microbial data suggest the presence of methanogens and methanotrophs in similar Fe and S reducing environments at both East and Slate River, CO sites. Researchers anticipate that the results will provide much needed quantification of hot spot and hot moment contributions to coupled BGC of redox-active and enzymatically important metals in relation to CH4 emissions in TAIs.

# Responses of Plant and Microbial Respiration Sources to Changing Cold Season Climate Drivers in the East River Watershed

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https://carbone-lab.nau.edu/index.php/ snodgrass-mountain-transect/

Global change is altering cold season climate in the western U.S. mountains. Snowpack is declining, snowmelt is occurring earlier in the spring, and growing seasons are becoming longer. This project will quantify the changing cold season climate effects on the soil carbon dioxide  $(CO_2)$  flux, and its plant and microbial sources in the East River Watershed, near Crested Butte, CO. Researchers are building on an exploratory grant, which established a network of soil CO<sub>2</sub> flux stations along an elevation gradient of different forest cover types. These measurements provide the foundation to use a model experiment (ModEx) approach to improve representation of belowground processes in mechanistic models. The team will install new automated soil CO<sub>2</sub> flux sensors designed to operate underneath the snowpack to expand measurements in cold seasons. Radiocarbon (<sup>14</sup>C) partitioning methods will be applied to determine how much of the soil CO<sub>2</sub> flux is coming from plant-root metabolism and microbial decomposition. Quantitative DNA stable isotope probing (qSIP) will be applied to quantify microbial community dynamics. Both <sup>14</sup>C and qSIP sampling will be purposefully scheduled in time and space to reduce the largest data-model uncertainties. Results from field studies will be applied to improve model parameterization and mechanistic representation of the soil CO<sub>2</sub> flux through plant and microbial mechanisms in FATES and MIMICS, respectively. The work is motivated by an overarching hypothesis that changing cold season climate drivers will impact belowground plant and microbial processes separately, and thus quantifying these influences is necessary to robustly predict how the East River Watershed ecosystems will respond to future environmental change. Researchers initial progress leverages long-term continuous dataset and machine learning approaches to assess how variability in snowpack, snowmelt timing, growing season length, and monsoon rain inputs influence the total soil CO<sub>2</sub> flux.

# Dynamics of Interconnected Surface-Subsurface Flow and Reactive Transport Processes Across the Hillslope-Riparian Zone River Corridor Continuum of Cold, High-Latitude Watersheds

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The Arctic is warming almost four times faster than the rest of the world and is in the process of thawing large stores of permafrost soil carbon (C). The conversion of soil C to greenhouse gases within watersheds is controlled by redox chemistry that is, in turn, controlled by how water flows through the soils from hillslopes to valley bottoms to streams. Watersheds are shifting in response to dramatic changes in extreme weather events like heat waves, flooding and storms, and more frequent wildfires, along with a shorter cold season and longer summer thaw season. The need is to improve models of cold-region watershed hydrology and biogeochemistry to predict how warming and permafrost thaw will affect greenhouse gas release in the future.

This research is integrating models of highly dynamic water flow over the landscape, through soils, and to rivers with key physical, biological, and chemical processes that control greenhouse gas generation and transport. Realistic coupling of the hydrology, biology, and chemistry in these models will be validated by key field observations. Expectations are that (1) hydrological flow patterns from hillslopes through valley bottoms control the landscape export of C from soils to rivers and the relative production of carbon dioxide versus methane; (2) variability in extreme events, freeze-thaw cycles, and day-to-day weather will alter the magnitudes of biological and chemical reactions through the hillslope to valley bottom and then to the river; and (3) watershed-scale C exports are controlled by valley-bottom processes, but hillslope and stream processes can dominate as climate change alters weather patterns and hydrology. Researchers will test these ideas under scenarios of shifting cold- and warm-season climate, by adding novel physics and chemistry to two coupled DOE models, the Advanced Terrestrial Simulator model for thermal hydrology and PFLOTRAN for reactive chemical transport.

# Reactive Transport Modeling of Iron-Sulfur-Carbon Cycling: Investigating The Impacts Of Dynamic Hydrologic Conditions at a Riparian Wetland

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Wetlands play a crucial role in enhancing water quality by transforming nutrients and organic substances, influencing the global carbon (C) cycle and greenhouse gas emissions, and retaining metals. Iron (Fe) flocs in the wetland can immobilize uranium (U), and the team hypothesizes that the presence of these flocs highly depends on Fe interactions with C and sulfur (S) in the hyporheic zone. Because spatiotemporally dynamic water fluxes promote fast redox cycling, net changes in S species are challenging to observe. Even when active, S cycling often remains hidden and thus overlooked in freshwater systems. The team's previous work has emphasized the importance of cryptic S reactions in Fe-S-C cycles under groundwater upwelling via two pathways: (1) anaerobic sulfide reoxidation (ASR) likely coupled to Fe<sup>3+</sup> reduction replenishes porewater sulfate  $(SO_4^{2-})$ ; and (2) anaerobic oxidation of methane (AOM) coupled to sulfate  $(SO_4^{2-})$  reduction moderates porewater methane  $(CH_4)$ , while methanogenesis buffers H<sup>+</sup>-consumption by Fe<sup>3+</sup> reduction. The team's current research further investigates the importance of cryptic S reactions under more complex hydrologic settings. Based on the observations at Tim's Branch, researchers implemented and compared reactive transport simulations with PFLOTRAN under three hydrologic flux scenarios: (1) constant flux; (2) regularly alternating flux direction; and (3) field-based dynamic flux. This model highlights the crucial role of cryptic S cycling in wetlands by increasing Fe<sup>2+</sup> and moderating CH<sub>4</sub> porewater concentrations. Moreover, this model indicates that dynamic hydrologic flux with alternating direction can facilitate increased Fe<sup>2+</sup> concentrations at different depths. When such an increase in Fe<sup>2+</sup> occurs at the sediment surface under upwelling conditions, it leads to the production of iron flocs in surface waters. These findings can help illuminate the impacts of dynamic hydrological settings on Fe-S-C cycles critical to carbon budgets and heavy metal mobilization.

#### Estimating Groundwater Recharge Across Mountainous Catchments

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This project reports on efforts to characterize and model deep groundwater system dynamics across a gradient of landscape and subsurface properties in montane to subalpine watersheds in west-central Montana and central Colorado. Multilevel groundwater wells have been installed in a variety of landscape positions and subsurface geology across the different watersheds. Borehole geophysics, core logging, and slug tests are used to characterize subsurface structure and hydraulic properties at drilling locations. Continuous water level and temperature logs are used to provide information on seasonal hydraulic dynamics. Environmental tracers (CFC, SF<sub>6</sub>, <sup>3</sup>H-<sup>3</sup>He, stable noble gas isotopes, stable isotopes of water) collected in wells and adjacent streams are used to provide information on timing, location, and volume of groundwater circulation. Researchers include new results of <sup>39</sup>Ar as a tracer capable of measuring intermediate

groundwater ages. These datasets are incorporated into conceptual and numerical models of integrated surface and subsurface flow to provide insight into the role of groundwater in hillslope and watershed behavior. Researchers find that mountains host active groundwater systems with strong seasonal responses to changing infiltration and evapotranspiration. Measured groundwater ages in these deep bedrock systems are characterized by a mixture of young and old water, with mean ages of 100 to 1,000 years. Models of surface and subsurface flow are highly sensitive to subsurface hydraulic characteristics, and specific subsurface configurations are required to fit the observed water table dynamics and groundwater mean ages. The deep critical zone including the saprolite and bedrock groundwater systems are an important, but often underexplored control on watershed hydrogeochemical function in mountainous systems. This project is producing new insight into the form and function of these hidden systems, and the role of deep, old groundwater in watershed function.

# How Does Wildfire Severity and Post-Fire Precipitation Influence Fate and Transport of Pyrogenic Organic Carbon and Nitrogen in Terrestrial-Aquatic Interfaces?

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Wildfires vastly disturb forest environments by influencing local hydro-biogeochemical cycles. The severity of a wildfire modifies the composition, transport, and abundance of pyrogenic organic matter (PyOM) in the natural environment, including pyrogenic organic carbon (PyOC) and nitrogen (PyON). Wildfire severity alters (1) the varying proportion of labile and soluble black carbon (BC) to recalcitrant and insoluble BC; (2) surface hydrodynamics of infiltration; and (3) known microbial community structure. Along with wildfire severity, postwildfire precipitation behavior further impacts the distribution of PyOM. Wildfire simulations at the watershed scale was conducted within the Clemson Experimental Forest (SC; Fall 2023) and is planned for Savannah River Site (SC; April 2024) to comprehensively document the influence wildfire severity and postfire precipitation have on the fate of PyOM across the terrestrial-aquatic interface. The production, composition, and fluxes of PyOM will be quantified in soil (particulate and porewater) and surface water samples (stream and runoff). The PyOM will be quantified by collecting soil and water samples before and after the wildfire simulation, natural precipitation events, and simulated rainfall experiments in locations of varying wildfire severity. Perturbations to watershed hydrodynamics due to the wildfires will be quantified through infiltration tests and soil saturation measurements. The leachability, degradability, and mobility of PyOM from soil and water samples will be quantified using controlled experimental conditions. The assessment of microbial community structures will determine their spatial and temporal relation to varying PyOM and nutrient pools, as well as their resilience and resistance to wildfire severity. The dissolved and particulate PyOM, nutrient pools, microbial structure, and hydrodynamic data obtained during field and laboratory experiments will be applied to develop a reaction network model and a reactive- transport model by coupling PFLOTRAN and ATS code. The field, laboratory, and modelling results aim to provide a mechanistic understanding of the natural hydro-biogeochemical response to varying wildfire severity and postfire precipitation.

# Molecular Features of Uranium-Binding Natural Organic Matter in a Riparian Wetland Using Ultrahigh Resolution Mass Spectrometry

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Tim's Branch riparian wetland, located in South Carolina, has immobilized 94% of the uranium (U) released >50 years ago from a nuclear fuel fabrication facility. Sediment organic matter (OM) has been shown to play an important role in immobilizing U. Yet, U-OM-mineral interactions at the molecular scale have never been investigated at ambient concentrations.

Sediment organic matter (OM) along the stream water pathway were extracted, purified, and concentrated. Molecular characterization was performed using Fourier transform ion cyclotron resonance mass spectrometry (FTICRMS). Out of 9,614 identified formulas, 715 contained U. These U-containing formulas were enriched with iron (Fe), nitrogen (N), and/or sulfur (S) compared to the entire pool of OM. Lignin-like and protein-like molecules accounted for 40% and 19% of the U-containing formulas, respectively. Phosphorus-containing formulas were found to exert an insignificant influence on complexing U. U-containing formulas in the mobile fraction (groundwater extractable) had lower nominal oxidation states of carbon (NOSC); lower N and S concentrations; and less aromatic moieties than the U-containing formulas recovered from the immobile fraction (sodium pyrophosphate extractable). U-containing formulas in the redox interfacial zones (stream banks) compared to those in nearby up-slope zones tended to have smaller molecular weights; lower NOSC; higher contents of COO and/or CONO functional groups; and higher abundance of Fe-containing formulas. Fe was present in 38% of the U-containing formulas but only 20% of the total OM formulas. It is postulated that Fe played an important role in stabilizing the structure of sedimentary OM, especially U-containing compounds. The identification for the first time of hundreds of U-containing formulas demonstrates the that the complexity of the system is much greater than commonly believed and numerically predicting U binding behavior in OM-rich systems should not be limited to measuring metal complexation with well-defined individual analogue organic ligands.

# Integrating Tree Hydraulic Trait, Forest Stand Structure, and Topographic Controls on Ecohydrologic Function in a Rocky Mountain Subalpine Watershed

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Predicting forest responses to climate change, requires understanding interactions among species differences in drought sensitivity, forest structure and landscape heterogeneity. Researchers are integrating these elements within a high-elevation watershed, using (1) field measurements of tree hydraulic traits, transpiration, canopy water content, tree ring-width variation, and soil moisture; (2) airborne observations of canopy temperature and water content; and (3) watershed-scale process modeling. Emerging results relate to a subset of the hypotheses:

• Rooting depth and stem capacitance explain differences in transpiration patterns across the watershed's **dominant tree species.** Preliminary results indicate significantly less negative xylem-P50 (xylem pressure at 50% loss of conductivity) for aspen versus the conifers. Spruce and pine, which have low sapflow, tightly regulate conductance, even at relatively high water potentials. Fir, which has high peak sapflow, releases more water from stem tissue than the other species. Aspen, which also has high transpiration, maintains flow with a low safety margin between stomatal-P50 and its xylem-P50.

- Across forest stands, radial growth covaries with topographic position. Preliminary results show that annual growth declines linearly with elevation and topographic position index for both spruce and fir, with lower growth at ridge positions. Growth is positively associated with relative moisture-retaining capacity of a site.
- Interannual differences in growth are smallest in convergent, high-elevation topographic positions with low incident solar radiation where the residence time of soil moisture is longest. Spruce growth is more sensitive to interannual precipitation variation and positively correlated with summer precipitation, while fir growth is inversely correlated with current and prior-year winter precipitation. This signal was strongest at high-elevation and convergent positions, suggesting that more and longer snow duration imposes energy rather than moisture limits to fir growth.

The team also demonstrate new simulation capabilities, using ParFlow-ELM-FATES to isolate the impact of subsurface lateral flow on evapotranspiration fluxes in complex terrain.

# Applying R-Osmos to Quantify Hot Moments in a High Mountain Watershed: Codevelopment of Novel Methodology to Advance Terrestrial-Aquatic Interface Models

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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 project will quantify the impact of hot spots and moments on microbial rates, focusing on two critical processes: methane (CH<sub>4</sub>) oxidation and nitrate  $(NO_3)$  reduction, at the DOE's East River Watershed Function Science Focus Area. For this project, researchers developed novel, continuous, time-integrating, in situ microbial rate samplers to inform the magnitude and variation in biogeochemical processes across the terrestrial-aquatic interface. In 2023, the team deployed these uniquely configured osmotic samplers (OsmoSamplers) to continuously quantify the rate at which microbial communities transform methane and nitrate on either side of a river meander. One of the packages was impacted by water level variation and was retrieved after a few months, however the second package (the downstream one), remains in place collecting data about the impact of meanders of river biogeochemistry. The remaining sampler package will be retrieved in early summer, which, after laboratory-based analysis, will allow the team to incorporate spatially explicit rate measurements of NO3 and CH4 oxidation and assimilation into reactive transport models developed for the region. Here, the team 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 Science Focus Area users.

#### Virtual

#### Seasonal Cycles Unravel Mysteries of Missing Mountain Water

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https://depts.washington.edu/mtnhydr/Pages/Research%20 Profiles/MissingWater.html

Snow provides over 60% of water supplies in the western United States, and in general, spring snow measurements provide a good prediction of summer streamflow. However, in some years, these streamflow predictions are not accurate, and water managers struggle to efficiently allocate water resources. In many studies, warming temperatures correspond to less observed streamflow per unit precipitation input. However, key elements, including basin heterogeneity, gauge undercatch, groundwater flow, and water storage, are often not represented in models or predictions, and physical hydrologic models diverge widely in their hydrologic sensitivity to warming. The project describes distributed observations in the well-instrumented East River (Colorado) and Tuolumne River (California) basins combined with modeling that researchers are using to investigate snow distribution as a function of elevation and snow

heterogeneity. The team hypothesizes that more uniformly distributed snow cover leads to greater subsurface water connectivity and more efficient water delivery to the stream. More variable snow cover, either through a greater elevational gradient or increased patchiness, leads to less effective recharge and greater evaporative losses. Only modeling that represents subsurface water transfer from snow-covered to snow-free grid cells will be able to represent these effects.

### Knowledge-Guided Clustering of Multidomain Data to Improve Predictions of Aerobic Respiration in River Corridors

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Thermodynamics-based biogeochemical modeling is increasingly popular, due to its ability to detail substrate chemistry and kinetics with a limited set of parameters. These models typically assume that all detected compounds are respirable, with degradation rates determined primarily by thermodynamic favorability. However, this assumption may not accurately reflect the complexity of data from diverse river systems, which contain differing microbial metabolic potential and growth rates in addition to substrate chemical and thermodynamic properties-all of which should influence whether a compound is respirable. In the team's previous analysis of high-resolution organic matter (OM) profiles from sediment samples collected as part of the Worldwide Hydro-biogeochemistry Observation Network for Dynamic River Systems (WHONDRS) Summer 2019 Sampling Campaign (Ahamed et al. 2023), the team identified interpretable key factors influencing OM bioavailability without accounting for sample-specific microbial traits. Therefore, in this work, researchers analyzed metagenomes and metadata from the same sampling campaign to better determine sample-specific microbial growth rates. The team filtered these additional features to those expected to directly influence respiration. Incorporating this data with the OM profiles, researchers have large data which spans physical, chemical, and biological contexts. To reduce complexity and extract interpretable findings, researchers performed dimensionality reduction on the chemical and metabolic features. The resulting principal components and physical data were used for clustering. Researchers were then able to account for environment-specific microbial traits by assigning distinct maximal growth rates among clusters, formerly assumed to be constant across samples. This analysis not only to improvements to predicted

respiration rates, but also highlights key drivers in diversity among microbial traits. As the next step, the team aims to incorporate this new knowledge into biogeochemical and reactive-transport models.

Ahamed, F., et al. 2023. "Exploring the Determinants of Organic Matter Bioavailability Through Substrate-Explicit Thermodynamic Modeling," *Frontiers in Water* **5**, 1169701.

#### Student

#### Groundwater-Dependent Fluxes of Water and Organic Carbon in a Permafrost Watershed Across Hydrologic States

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Suprapermafrost aquifers within the active layer are present in the Arctic during summer. The exacerbated permafrost thaw rate due to global warming in the Arctic will liberate previously frozen particulate organic matter (POM). The POM leaches dissolved organic carbon (DOC), which gets transported through groundwater flow. How much DOC is delivered by groundwater into surface water remains uncertain. This input is critical to landscape budgets and for predicting the long term fate of carbon. The team quantified groundwater and DOC fluxes into a representative headwater stream of a continuous permafrost watershed-the Imnavait Creek (IC) in Alaska. This was done across thousands of scenarios represented by steady groundwater flow simulations based on high-resolution topography combined with aquifer transmissivity and DOC data. The predicted groundwater discharge values, which represent all possible hydrologic conditions excluding the freshet, are similar to and span the range of IC streamflow. Researchers also found that IC's DOC may be entirely sourced from groundwater. Thus, riverine and lacustrine ecological and biogeochemical processes relate strongly to groundwater phenomena in these continuous permafrost settings. As the Arctic warms and the active layer deepens, it will become more important to understand and predict suprapermafrost aquifer dynamics.

#### Feedback Loops and Abiotic Determinants of Biomass Growth and Its Impact on Chromium Reduction in the Hyporheic Zone

Marc Berghouse, Rishi Parashar\*

Late addition. See full abstract, p. 109

#### Constraining the Timing and Tempo of Clay Mineral Formation and Organic Matter Stabilization in an Alpine Watershed: East River, Colorado, United States

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Soil organic carbon (OC) constitutes the largest terrestrial pool of carbon, and changes in its size have the potential to modulate atmospheric CO<sub>2</sub> levels. As such, the underlying controls on OC stabilization and their sensitivities to climatic change have been increasingly scrutinized. The existing paradigm for OC stabilization suggests that due to their high specific surface areas and negatively charged surfaces, secondary clay minerals that form in soil protect OC from oxidation. Thus, a direct relationship between clay mineral abundance and OC may hold across soil types and climates. Despite this understanding, reactive transport models (RTMs) cannot reconcile soil geochemistry and OC profiles, pointing to knowledge gaps regarding organo-mineral interactions and their constitutive controls. Consequently, these challenges result in great uncertainty in the treatment of soil OC dynamics in Earth systems models and their concomitant effects on future climate projections.

To further understand clay mineral formation and its relationship with OC dynamics over a hydrologic year, the team first interprets published river solute data from the East River Watershed, CO. Numerical couplings will help validate these preliminary findings.

#### Student

#### Bald Cypress Knees Contribute to Methane Emissions in a Bottomland Hardwood Wetland

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Relatively little is known about carbon source-sink dynamics in bottomland hardwood wetlands. Identifying carbon pathways and their dominant controlling factors within these systems is critical. Bald cypress (*Taxodium distichum*) is a dominant tree species of southeastern United States wetlands. These trees can develop exposed woody root structures known as knees, which have been shown to contribute to wetland methane (CH<sub>4</sub>) emissions. However, there are significant variations in estimates of knee contribution to total ecosystem flux. The team is measuring variation in  $CH_4$  and carbon dioxide  $(CO_2)$  fluxes from individual knees, soils, and 1 m<sup>2</sup> plots containing both soils and knees as a function of microtopographic and climatic (i.e., drought and flooding) differences. During moderate-severe drought conditions in the autumn of 2022, knees acted as a source of CH<sub>4</sub> even while their surrounding soils acted as a sink. Soil CO<sub>2</sub> emissions were significantly related to surrounding knee density during drought conditions (p-value=0.0374), but no relationship was found between soil CH<sub>4</sub> uptake and knee density. Similarly, in 1 m<sup>2</sup> plots, there was no clear relationship between knee density and CH<sub>4</sub> and CO<sub>2</sub> flux. During nondrought conditions, in the autumn of 2023, researchers saw an increase in CH4 emissions from individual knees but only from those located at a lower elevation. A historic rainfall event (dropping 17.7 cm of precipitation in 24 hours) in July 2023 also resulted in an approximately 250% increase of CH<sub>4</sub> emissions from knees at the lower elevation. The flooding and drought period data suggest fluxes are partially related to hydrologic factors. Sampling is ongoing to better understand the relationships between knee fluxes and surrounding environmental factors (i.e., hydrology, air and soil temperature, soil biogeochemistry). This allows for more accurate wetland ecosystem carbon modeling, which currently does not account for knee fluxes.

#### Student

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

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Northern Arizona University, Flagstaff, AZ

https://carbone-lab.nau.edu/index.php/ snodgrass-mountain-transect/

Mountainous ecosystems in the western United States are experiencing substantial changes in their water inputs with the dominant water source—snowpack—decreasing and melting earlier, and monsoon rains becoming more sporadic. In these ecosystems, there is a lack of understanding of how belowground soil carbon production  $(CO_2 \text{ flux})$  will respond to these changes in precipitation inputs. This is in part due to the logistical difficulty of conducting fieldwork in these ecosystems' complex terrain, as well as the technical challenge of separating the two components of the  $CO_2$  flux, root, and microbial respiration. This research aims to understand how precipitation inputs influence root and microbial respiration individually by conducting an intensive radiocarbon sampling campaign paired with long-term continuous measurements of the CO<sub>2</sub> flux and its primary environmental and biological drivers (soil temperature, soil water content, and plant productivity). During the summer of 2022, the team conducted four different field visits over 24 days at long-term environmental monitoring sites in the East River Watershed of Colorado. Samples collected included manual CO<sub>2</sub> flux, soil water content, and soil temperature. These measurements were used to constrain and validate the continuously measured CO<sub>2</sub> flux at these sites. During the July-September sampling, Simonpietri collected more than 150 radiocarbon samples to separate root from microbial respiration through isotopic partitioning. Simonpietri processed each of these samples (1 hr sample-1) by purifying them to  $CO_2$ , then graphitizing and pressing them into aluminum capsules to be run on the accelerator mass spectrometer. The primary findings from this research show that root and microbial respiration have different environmental sensitivities throughout the growing season.

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

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Hydrological processes in riparian and hyporheic sediments create strong biogeochemical gradients and redox microniches that are metabolically influenced by temporal changes in precipitation, temperature, and stream discharge. The complex temporal and spatial variability of these processes and their effect on the transformation and exchange of carbon (C), nutrients, and greenhouse gases (GHGs) with surface waters are difficult to account for in reactive transport models. 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. In this project, state-of-the-art in situ physical and geochemical measurements are combined with metaomic signals of the active microbial populations in riparian and hyporheic sediments of Steed Pond at the Savannah River National Laboratory

to predict the role of hydrological forcing on the spatiotemporal transformation of C, nutrients, redox processes, and GHG emissions along this gaining and losing wetland stream. During Year 3, the data from two in situ electrochemical systems that monitored the temporal variations in pore water redox biogeochemistry at both a gaining and losing reach were correlated with monitoring well water levels and rainfall to determine how redox processes in the hyporheic zone are affected by hydrological forcing. In addition, the production of methane  $(CH_4)$  in streambed sediments was compared to CH<sub>4</sub> benthic fluxes measured simultaneously to investigate the role of vegetation in net GHG emissions under both gaining and losing conditions. In parallel, metagenomic signals from sediment slurry incubations designed to investigate the competition between anaerobic microbial processes in hyporheic sediments were analyzed using Pacific Northwest National Laboratory's supercomputer COMPASS to identify the main microbial metabolic processes under various geochemical conditions. Finally, the main redox geochemical processes involved in the transformation of carbon were incorporated in the reactive transport model PFLOTRAN in both 2D and 1D to investigate how gaining and losing conditions affect redox processes. Along with the high spatial and temporal resolution of biogeochemical processes, the developed numerical models will predict how variations in hydrological forcing, competition between microbial metabolic processes, and porosity changes associated with biogeochemical feedback affect C and nutrient cycling as well as GHG emissions.

# Investigating Hydrologic Connectivity as a Driver of Wetland Biogeochemical Response to Flood Disturbances

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#### http://ecohydrology.ua.edu/projects.html

Wetlands serve as biogeochemical control points, regulating nitrogen (N) removal from local to watershed scales. Flood disturbances influence wetland biogeochemical activity by delivering dissolved organic matter (DOM) and nutrients to wetland soils. This delivery is regulated by the mode of hydrologic connectivity (i.e., hillslope-connected vs. floodplain-connected flowpaths) to the stream. However, researchers lack an understanding of how differences in flood-driven water and material delivery affect post-flood biogeochemical processing within wetlands. The objective of this study is to determine how hydrologic connectivity mediates wetland biogeochemical response to floods at a forested, headwater coastal-plain system. Researchers designed the project to adhere to Integrated, Coordinated, Open, and Networked (ICON) science principles.

Wetland water-level measurements show increasing inundation durations from hillslope-to-floodplain wetlands. Researchers have installed additional piezometers to empirically measure the surface water and groundwater water levels of the wetlands and the surrounding upland, which can be used to examine the solute dynamics from a hydraulic gradient. Potential denitrification and dissimilatory nitrate reduction to ammonium (DNRA) rates in wetland soils varied between individual wetlands but were overall higher during the wet season. The team will use inundation duration and frequency of saturation events to further elucidate drivers of potential nitrate reduction pathways.

Researchers used the Advanced Terrestrial Simulator (ATS) to model subsurface, surface, and canopy water in a comparable small, forested wetland, and found that hydrogeomorphology drives reach-scale patterns of water availability and drying. The next goal is to use PFLOTRAN to model biogeochemical cycling in an individual wetland. To provide empirical measurements of watershed carbon and nitrogen export, a water quality sensor probe will be deployed at the watershed outflow. Overall, initial findings indicate that seasonal (i.e., wet vs. dry) drivers play an important role in regulating wetland and watershed nutrient processing across the gradient of hydrologic connectivity.

# Linking Root and Soil Microbial Stress Metabolism to Watershed Biogeochemistry Under Rapid, Year-Round Environmental Change

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

Air temperatures are rising causing the winter snowpack to shrink, thereby increasing soil freeze-thaw events in high latitude ecosystems. This project focuses on understanding the shifts in microbial metabolism of soil carbon (C), nitrogen (N), and phosphorus (P), which are the mechanisms that underlie exports at the watershed-level. Researchers are conducting a model-data integration study using the Climate Change Across Seasons Experiment (CCASE) at the Hubbard Brook Experimental Forest (HBEF). At CCASE, replicate field plots receive one of three climate treatments: (1) growing season warming (+5°C above ambient); (2) warming plus freeze-thaw cycles  $(+5^{\circ}C \text{ above})$ ambient in growing season plus up to four freeze-thaw cycles in winter); and (3) reference conditions (no treatment). The team found that warming plus freeze-thaw cycles induce redox stress and select for anaerobic N-cycling microbes. Researchers are working to couple these microbial shifts with changes in the belowground N pool and flux measurements in organic and mineral soil horizons collected over the past decade. The team aims to incorporate both immediate and evolved responses of microbial C, N, and P cycling into new versions of an ecosystem model (PnET-BGC). This research tests conceptual understanding of plant and microbial physiological 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.

#### Student

#### Microbial Metabolisms Connecting Iron and Carbon in Terrestrial Wetlands: A Metagenomic and Metatranscriptomic Study of the Savannah River Site

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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 iron oxidation and its connection to carbon cycling and to incorporate these metabolisms into hydro-biogeochemical models, one needs to know the rates and mechanisms of biotic and abiotic oxidation. To evaluate this, the team conducted two SRS field campaigns to sample iron mats in the Tim's Branch stream and wetlands. Researchers performed 16S rRNA gene sequencing to identify the major iron-oxidizing bacteria (FeOB) and the flanking community, and metagenomic sequencing to identify the major biogeochemical transformations catalyzed by FeOB metabolisms.

Additionally, researchers performed iron oxidation kinetics experiments to quantify biotic iron oxidation rates, connected to metatranscriptomics sequencing to identify the expression of metabolic pathways in response to Fe(II) stimulus. The iron mats were dominated by known FeOB, notably a diverse set of *Gallionella* and *Leptothrix* taxa. Scanning electron microscopy shows the major morphologies in the mats are FeOB biominerals, including twisted stalks (characteristic of Gallionella) and sheaths (characteristic of *Leptothrix*). The team compared biotic oxidation rates with abiotic azide-killed controls and showed that mat iron oxidation is dominated by biotic oxidation while oxidation by abiotic mechanisms was much slower. Researchers will present the results of metagenomic and metatranscriptomic analyses of the Fe mat communities used in the kinetics experiments, including the major physiological mechanisms of the dominant FeOB. Researchers will describe the biogeochemically relevant activities of all major iron mat community members, detailing the metabolic links between iron oxidation and carbon metabolisms, and outline the major interactions between taxa. These results set the stage for microbial modeling work towards the longer-term goal to link FeOB metabolic models and kinetics to biogeochemical models in order to predict iron, carbon, nutrient, and contaminant metal cycling.

#### Virtual

#### The QuEST Project: Integrating Catchment Expansion-Contraction Dynamics into Cross-Continental Hydro-Biogeochemical Predictions

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The QuEST (Quantifying Ecosystem exports across Space and Time) Project seeks to expand understanding of hydrologic and biogeochemical change in headwater networks that dynamically expand and contract. Headwater stream networks comprise approximately 80% of all river miles on Earth and are important "reactors" due to their relatively large reactive streambed surface area as compared to the volume of water and materials they transport. The transformations and transport of materials in headwater streams reflect multiple upslopes and within-stream material sources and ecological processes. Climate-mediated changes in patterns of stream network expansion and contraction in response to shifting precipitation regimes have the potential to interact with material processing within headwaters and change material export to larger rivers. Researchers currently lack a predictive understanding of these complex interactions and how they may alter surface water quality, habitat sustainability, and drinking water security across the United States. The project's approach integrates hydrologic modeling with

complementary hydrologic and biogeochemical observations within five watersheds spanning the United States' cross-continental aridity gradient. Specific activities include (1) integrating empirical data and hydrological models to evaluate surface and subsurface flow contributions to the flowing structure of the stream network, (2) using comparative ecohydrological metrics from repeated snapshot campaigns of catchment-wide stream chemistry to evaluate how small headwater tributaries impose variability observed at coarser spatial scales, and (3) deploying an array of highfrequency water quality sensors spatially distributed within each catchment to capture how stream network expansion and contraction dynamics change carbon, nutrient, and material exports across climatic conditions. As data collection occurs, researchers are also analyzing existing long-term datasets to address the project's central questions and characterize the focal watersheds. The team will present the project's structure and goals as well as preliminary results from initial field campaigns and ongoing analyses.

# Impacts of Streambed Dynamics on Nutrient and Fine Sediment Transport in Mountain Rivers

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In mountainous watersheds, rivers typically have armor layers of coarse sediment that protects the finer subsurface from erosion. In theory, armor layer motion during high flows could release 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 location is losing or gaining.

Researchers tested whether armor layer motion and streambed concentrations influence hysteresis patterns during summer monsoon and snowmelt flows in La Jara Creek in Valles Caldera National Preserve, NM. Before flow events, the team sampled streambed concentrations of POC, PP, SRP, and fine sediment and installed streambed baskets to capture SS deposition. During high flow events, researchers measured (1) surface and groundwater exchange at local (basket) and reach scales; (2) timing of armor layer motion; and (3) river concentrations of POC, PP, SRP, and SS. The team also conducted experimental floods to isolate the role of armor layer motion on these constituent concentrations in the water column.

Preliminary results suggest that the quantity of fine sediment captured in streambed baskets was related to the local hyporheic flux and near-bed flow velocity. SS, turbidity, PP, and POC often followed the same hysteresis pattern in each natural flow event, suggesting that they may have a similar source. During experimental floods, in which armor layer motion was the only source of particulate matter, hysteresis of SS and PP occurred. The timing of armor layer motion may have also controlled different observed constituent hysteresis patterns between natural flow events.

Researchers are currently investigating potential hysteresis sources during these events and constraining the exact timing of armor layer motion in each event.

# Groundwater Supported Vegetation Refugia as a Mechanism of Forest Recovery in a Rocky Mountain Watershed Impacted by Disturbances

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Groundwater can form consistently wetter land surface areas to support greater ecosystem productivity across scales and climate zones. The research team examined the conditions under which groundwater facilitates forest recovery after disturbance(s) in the Medicine Bow National Forest (MBNF) where logging, bark beetle, and wildfire disturbances occurred in recent decades. For a 40x25 km<sup>2</sup> area spanning subalpine to montane forests, field surveys revealed that groundwater-supported forest refugia (GSFR) occur along the entire elevation gradient in the form of forested/shrub wetlands, springs, and perched aquifers (Zhang et al. 2023). These features have sheltered trees against one or more disturbances although seed-bearing trees can facilitate forest recovery only if water table is of suitable depth, is persistent, and in the case of wildfire, soil and seeds remained viable after the fire. GSFR can change over time, driven by feedback between disturbance, vegetation response, and hydrology: at a forested and shrub wetland, a 2020 wildfire that burned surrounding uplands may have resulted in a raised local water table that stressed formerly healthy trees in the wetland, casting doubts about its future refugium status. These field observations are being tested at site and landscape scales using a coupled ecohydrological model calibrated against historical and new measurements (i.e., colocated climate, vegetation, soil moisture, and

groundwater data). Simulation results suggest (1) for a subalpine wetland and upland site, understory growth must be represented to accurately model post-beetle-kill recovery; (2) at the landscape scale, high average soil moisture surrounding GSFRs maintained evapotranspiration and gross primary productivity during a drought year while the latter half of the growing season saw greater growth; and (3) at both scales, water and light were the limiting factors affecting the growth and survival of tree seedlings. The team will implement a new competition scheme into the model, enabling the seedlings to compete for water and light with coexisting shrubs, grasses, and forbs.

Zhang, Y., 2023. "Forest Recovery After Disturbances Facilitated by Groundwater: A Study at the Medicine Bow Mountains in Southeastern Wyoming," Colloquium, Department of Geosciences, University of Montana.

# Watershed Sciences National Laboratory-Led Projects

# BioGeoChemistry at Interfaces Science Focus Area

The Lawrence Livermore National Laboratory BioGeoChemistry at Interfaces Science Focus Area: A 15-Year Effort to Identify Biogeochemical Processes Controlling the Fate of Radionuclides in the Environment

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https://ess.science.energy.gov/llnl-actinides-sfa/

Originally titled the Plutonium Science Focus Area (SFA), the focus of the BioGeoChemistry at Interfaces SFA for the

past 15 years has been to identify and quantify the biogeochemical processes and the underlying mechanisms that control the mobility of actinides and other redox sensitive elements in an effort to reliably predict their cycling and migration in the environment. The research focus shifted over the years from detailed mechanistic laboratory studies of intrinsic Pu colloid formation using molecular modeling and atomistic spectroscopy and microscopy to field-scale characterization of long term (>decadal) cycling of radionuclides and trace elements in a series of test beds located across the U.S. (and U.K.). The investment of BER in this SFA program allowed the SFA team to adjust its research focus over time to answer critical questions that limit the ability to predict the long term fate of contaminants associated with DOE's (and the world's) most complex radiochemically contaminated environments. Throughout its history, this SFA was founded on three research pillars: (1) Field Studies that capture biogeochemical redox processes on the timescale of decades; (2) Fundamental Laboratory Studies that isolate specific biogeochemical processes observed in the field; and (3) Harnessing the unique capabilities and staff expertise at Lawrence Livermore National Laboratory and its national laboratory partners to advance the understanding of biogeochemical redox processes in the environment and serve as an international resource for environmental radiochemistry research.

The SFA concept within BER is structured for conducting coordinated, team-oriented research in a manner that is distinct from, but complementary to, BER-supported research conducted via individual, single-investigator projects at other institutions. This approach challenges the DOE national laboratories to build and sustain integrative, team-oriented research programs based on their unique scientific capabilities and administrative resources to meet the strategic goals of the ESS program. Over its successful and productive 15 year history, the Biogeochemistry at Interfaces SFA has led to publication of over 70 manuscripts with approximately 175 co-authors, innumerable presentations at national and international conferences, the ACS Francis P. Garvan-John M. Olin Medal received by the original Principal Investigator (Annie Kersting) that recognized her distinguished service to chemistry, and the development of a robust pipeline of next-generation radiochemists into the national Laboratories and U.S. universities.

#### Long-Term Transport of Radionuclides in Watersheds: Case Studies from Three Test Beds

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#### https://ess.science.energy.gov/llnl-actinides-sfa/

While much progress has been made in the mechanistic understanding of geochemistry of radionuclides, there are still gaps in knowledge regarding their long-term mobility in surface and subsurface environments. The Biogeochemistry at Interfaces has established three test beds at Savannah River Site (SRS), Nevada National Security Site (NNSS), and Hanford Site with different contamination histories, climate, hydrology, and geology to study these processes.

Pond B, a monomictic reservoir, at SRS received cooling water from the R-reactor, which resulted in low-level contamination of anthropogenic radionuclides plutonium (Pu) and caesium-137 ( $^{137}$ Cs). Two consecutive years of monitoring demonstrated the occurrence of highly correlated concentration profiles of arsenic, iron, aluminum, plutonium, and dissolved organic matter, all of which increased in concentration by 1 to 2 orders of magnitude within the anaerobic hypolimnion.

Plutonium appears to have become incorporated into the natural iron and carbon cycles with the highest concentrations in water observed at the start of stratification, with the majority released from shallow waters associated with Fe(III)-particulate organic matter.

In contrast to the saturated Pond B system, researchers studied radionuclide transport in an ephemeral wetland at NNSS. Over the last 65 years, the E-Tunnel ponds have continuously collected groundwater discharging from a tunnel where several underground nuclear tests were conducted from the 1950's to the 1970's. Variably saturated pond sediment profiles of Pu and <sup>137</sup>Cs show that Pu remains immobilized, but <sup>137</sup>Cs is largely lost from the pond sediments. Future column experiments will explore the mechanisms behind radionuclide (im)mobilization under wet-dry cycles.

The Z-9 trench vadose zone at Hanford was contaminated with a comparatively larger amount of radionuclides (e.g., ~40 to 150 kg Pu) in an acidic waste containing organic processing solvents. In an effort to better understand Pu migration below the Z-9 trench, researchers undertook a series of bench-scale saturated column experiments using uncontaminated Hanford sediments and Pu in a range of high nitrate, acidic solution compositions with and without TBP in dodecane. These results of this study show that Pu migration is likely driven by weak sorption of aqueous Pu under low pH conditions as well as the formation of Pu-TBP-nitrate complexes in the organic phase at pH < 4. Pu migration in the subsurface will be limited by the natural buffering capacity of the sediments as well as the dispersal of the nitrate plume.

#### **River Corridor Science Focus Area**

#### River Corridor Science Focus Area: The Next Evolution

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

The next evolution of Pacific Northwest National Laboratory's (PNNL) River Corridor science focus area (SFA) will deliver the knowledge, models, and data needed to quantify, understand, and predict how watershed perturbations and biophysical settings combine to drive water and material transport into, perturbations within, and cumulative biogeochemical function of sediment-associated components of stream networks. Researchers take a systems approach to reveal how watershed hydro-biogeochemical processes lead to emergent function. Over the next quadrennial period researchers will reveal how variation in the physical, chemical, and biological attributes of watersheds (i.e., biophysical setting) interacts with watershed perturbations (e.g., wildfire) to drive perturbations occurring directly within stream networks (e.g., loss of surface water), and how that collection of interconnected processes leads to stream-networkscale sediment respiration rates.

Spatiotemporal patterns of sediment respiration (ERsed) is an emergent property of watershed systems that arise from interacting, non-linear processes distributed throughout watershed systems. Researchers focus on ERsed because its contribution to carbon cycling in stream networks range from being the dominant driver to being inconsequential. This variation has not been broadly quantified, understood, or predicted. Further, the ability to understand and predict spatiotemporal patterns of ERsed provides a litmus test for the quality of the predictive understanding of integrated watershed processes. Wildfire and the loss and gain of surface water (i.e., variable inundation) are the focal perturbations external to and within stream networks, respectively. The team focus on these together because they can interactively influence ERsed via physical, chemical, and biological processes. Further, wildfire is becoming more common, higher intensity, and burning larger fractions of watersheds, while variable inundation is, arguably, the most ubiquitous perturbation experienced by Earth's stream networks. The team will use an integrated research program distributed across basins and founded on a watershed systems approach to test hypotheses and resolve knowledge gaps associated with the impacts of perturbations on emergent properties.

#### Watershed Ecohydrological Responses to Disturbances Under Changing Climate

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#### https://www.pnnl.gov/projects/river-corridor

Disturbances such as wildfire, insect outbreaks and droughts cause significant but poorly understood impacts on water and carbon cycles, posing an unpredictable threat with increasing frequency, spread, and severity of disturbances. It is crucial to comprehend post-disturbance recovery processes in watersheds to elaborate the understanding of disturbance impacted ecohydrological processes and the implications of changing climate. Thus, researchers investigated climate, topography and fire impacts on recovery responses in burned areas that occurred in 2015 across the Columbia River Basin. Using the Enhanced Vegetation Index (EVI) as a proxy of post-fire vegetation biomass recovery, random forest (RF) models were trained for each land cover type to quantify the relationships between incremental EVI recovery and various climate and biophysical factors, including annual precipitation, annual median maximum daily temperatures, elevation, slope, aspect, burn severity and years elapsed after fire. Feature importance analyses revealed that precipitation and temperature were the two most influential factors controlling the EVI recovery. Partial dependence analyses revealed that increasing precipitation was associated with increasing incremental EVI changes for all land cover types.

Evergreen forest showed increasing EVI change with increasing temperature. Conversely, shrubs and grassland showed rising trends in EVI until reaching 12.5°C, above which a reverse trend was observed. This work is an important step towards understanding and representing ecohydrological responses to disturbances. While current work explores vegetation recovery using remote sensing products, the next step is to employ vegetation dynamics model ELM-FATES to account for post-fire vegetation recovery and its impact on water, energy, and carbon budgets. ELM-FATES can be further coupled with ATS-PFLOTRAN to enable the integration between ecohydrologic and hydro-biogeochemical processes from the hillslopes to watersheds, providing new insights into water and carbon export from land to streams as impacted by the interactions among watershed biophysical setting, climate, and disturbances.

#### Multi-Basin Modeling, Regional Transferability, and Hypothesis-Based Model-Experiment (ModEx)

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The hyporheic zone (HZ) plays a major role in the hydrological and ecological function of river ecosystems. While lab, field, and numerical studies have improved the understanding of the underlying biogeochemical processes in HZ, scaling up to reach and network scales or transferring this knowledge between basins remains a challenge due to modeling, observation, and scaling limitations. Researchers address these challenges using a hypothesis-based modelexperiment (ModEx) loop leveraging the coupled river corridor model (RCM) to quantify HZ aerobic and anaerobic

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respirations. Key factors controlling their spatial variability within the Columbia River Basin were then identified via machine learning (ML). These results show that riverbed carbon dioxide  $(CO_2)$  emissions vary with sub-basin drywet conditions, river sizes, and oxygen availability, and most of the spatial variation can be explained by the hydrological exchange fluxes (HEFs), which further depend on streambed grain size. Due to the importance of grain size, a photo-driven, artificial intelligence (AI)-enabled, and theory-based framework was developed to quantify grain sizes and hydro-biogeochemical parameters from photos. The AI is trained with around 12,000 grain labels representing nine typical stream environments using a state-of-theart computer vision AI with a Nash-Sutcliffe-efficiency of 0.98 and relative error of 6.7%. The team applied the AI to extract streambed grain size distributions from photos collected across the Yakima River Basin, and to existing grain size datasets from USGS, NEXSS, and other ML-derived products to better understand how this approach can help bridge data gaps in grain size information across watersheds. Finally, it was assessed whether hyporheic respiration scales allometrically with watershed area, and whether relationships can be generalized within and across basins. Researchers found consistent relationships between allometric scaling, HEFs, and watershed elevation, suggesting their potential to generalize these relationships to basins where HZ respiration has not, or cannot be modeled.

#### Reconciling Variation and Interconnections in Stream Network Organic Matter Degradation and Microbial Community Activity Across Scales

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#### https://www.pnnl.gov/projects/river-corridor

Substantial amounts of dissolved organic matter (DOM) are transported throughout river ecosystems and undergo abiotic and biotic interactions with the surrounding ecosystem. Despite this importance, researchers know little regarding the spatial scaling of DOM or the microbial communities degrading it. To investigate these concepts, researchers leveraged high-resolution DOM characterization, microbial sequencing, and novel data science approaches. The team observed linear relationships between stream size and both DOM functional diversity and the number of potential biochemical transformations in the Yakima River Basin (YRB). Results from five other watersheds revealed that, while the types of relationships observed in the YRB were not universal, catchment-specific spatial variables were significantly related to transformation count indicating spatial scaling patterns for DOM. A machine learning approach was used to investigate the bioavailable component of DOM and indicated that thermodynamic favorability, the number of carbons, and carbon-to-nitrogen ratios were important molecular formula properties when predicting respiration rates. Researchers combined DOM characterization data with shotgun sequencing and identified putative connections between microbes and DOM at the continental U.S. (CONUS)-scale. The team identified 2093 unique metagenome assembled genomes belonging to 27 phyla and found that microbial metabolism became dominated by clades capable of using simple carbon compounds as watersheds increased in size. These studies revealed that DOM has spatial scaling connected to land cover and stream size while the microbial communities more closely mirrored predictions posited by the River Continuum Concept.

#### Hypothesis-Based Model-Experiment (ModEx) Reveals Effects of Drivers and Disturbances on Basin-Scale Ecosystem Respiration

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

River corridors emit significant amounts of carbon dioxide  $CO_2$  to the atmosphere through both abiotic and biotic processes. Biotic CO<sub>2</sub> contributions (i.e., ecosystem respiration) from different riverine components (e.g., benthic, hyporheic, water column) are highly variable and poorly understood at basin scales. Researchers use hypothesis-based model-experiment (ModEx) to increase mechanistic understanding of ecosystem respiration within and between river corridor components and extend these mechanisms into conceptual models including disturbance effects at the basin-scale. The first ModEx cycle used River Corridor model outputs to hypothesize basin scale drivers of ecosystem respiration and design field experiments to test those hypotheses. Researchers evaluated whether the spatial variation in model-predicted deep hyporheic respiration explained spatial variation of field observed ecosystem

respiration rates. The team found no correlative relationship between the predicted and observed rates; thus, researchers explored additional mechanisms studying the contributions from water column and sediment-associated components. This ModEx cycle revealed that sediment-associated respiration, excluding deep hyporheic zone respiration, are the primary drivers of spatial variation in ecosystem respiration in the testbed basin. A second ModEx cycle investigated the effects of wildfire disturbance on ecosystem respiration. Researchers first coupled field observations with a recently developed fire module of the SWAT model to evaluate how watershed function may be impacted by changing burned area and severity. Model simulations suggested that high burn severity led to the greatest increase in nitrate while moderate burn severity led to the greatest increase in dissolved organic carbon concentrations.

Researchers then designed a field campaign to test how these post-fire water quality changes could impact ecosystem respiration in fire impacted systems across different periods of hydrologic connectivity in the testbed basin. Together, the hypothesis-based ModEx cycles uncovered landscape predictors and mechanisms modulating ecosystem respiration at the basin scales, enabling hypothesis testing and model improvements not otherwise possible.

### Integrating Organic Matter Measurements into Watershed Hydro-Biogeochemical Models

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#### https://www.pnnl.gov/projects/river-corridor

Watersheds play significant roles in modulating carbon and nitrogen cycling and removal of excess nutrients. The incorporation of molecular-level characteristics of organic matter (OM) from field measurements is expected to greatly improve the ability of watershed hydro-biogeochemical models to capture distinct water quality and quantity signatures under disturbance, thus facilitating iterative coupling with field measurements under model-experiment (ModEx) framework. However, the connections between OM measurements and biogeochemical reaction network from batch to watershed scales are missing. Researchers developed an integrated modeling approach that links site-scale OM chemistry measurements to watershed-scale modeling. At the site scale, a Python workflow was developed to connect OM chemistry informed by high-resolution Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) into an aerobic respiration simulator using the PFLOTRAN reaction sandbox. Moreover, to account for the role of non-oxygenic electron acceptors in regulating organic matter turnover and the fate of carbon, researchers expanded the aerobic respiration-based carbon speciation by incorporating both detailed OM chemistry and electron acceptors other than oxygen. At the watershed scale, researchers developed an integrated model that couples the formulated site-scale batch reaction in PFLOTRAN with a distributed flow and transport model ATS. Researchers have employed ATS to study the impact of wildfire disturbance on watershed hydrological response by implementing a new fire module to modify the soil properties in fire scars. Researchers demonstrated the usage of the watershed model to evaluate the downstream runoff to wildfires across multiple watersheds in Pacific Northwest, such as Naches River Watershed. To further study disturbance impacts on watershed biogeochemistry, future work will: (1) incorporate the generalized carbon speciation method into the Python workflow; (2) enable characterization of spatiotemporal variation of reaction networks in watershed models; and (3) leverage additional advances the team has contributed to, such as the omics-to-reactive-transport pipeline that explicitly links microbial genomics to PFLOTRAN.

#### Wildfire Influences on Stream Network Hydro-Biogeochemistry Are Related to Watershed Properties, Burn Severity, and Organic Matter Chemistry

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#### https://www.pnnl.gov/projects/river-corridor

Wildfires impact river corridor hydro-biogeochemical function by altering the availability of organic matter (OM) and nutrients within the landscape and the hydrological mechanisms responsible for their delivery to aquatic systems. A shift in post-fire input to aquatic systems can have cascading impacts on carbon and nitrogen stoichiometry that may impact stream metabolism. Developing a predictive understanding of wildfire impacts remains a challenge, due to the complex array of spatial and temporal drivers that influence stream biogeochemistry post-fire. To better understand localized drivers of dissolved organic carbon (DOC) concentrations across a stream network, researchers used a Spatial Stream Network (SSN) model to study a stream network impacted by fire with ~100 sites above, within, and below the burn perimeter across seasons. The SSN model indicated that wildfire impacts were masked by the variability of site-level landscape characteristics across the watershed. During dry periods burn severity was not a major influencing factor, but as the basin seasonally rewet, burn severity did influence observed DOC concentrations, showing a decrease in DOC with increasing burn severity. In streams with drainage areas entirely within the burn perimeter, the spatial drivers of OM chemistries (e.g., burn severity) were partially modulated by localized hydrological processes. Researchers have also found that thermodynamically predicted bioavailability of fire-altered OM may be higher than previously assumed. Together, these results suggest that spatiotemporal controls on the transport of fire-altered OM to the stream network influence in-stream biogeochemical processes, highlighting complexity in upscaling localized watershed scale processes across systems and scales. Confirming this complexity, researchers found that relationships between DOC, climate, and percentage of watershed burn area in fire impacted systems exhibited high spatial variability across the continental U.S. Collectively, this work has advanced the understanding of wildfire impacts on DOC quantity and OM quality post-fire, with implications for aquatic ecosystem function.

#### Beyond Data Assimilation: A Hypothesis-Driven Model-Experiment (ModEx) Approach to Predictive Modeling of Sediment Respiration Across the Continental United States

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

Hyporheic zones play a dominant role in the metabolism and biogeochemistry of river corridor systems. Hyporheic sediment respiration exhibits high spatial variability within and across river basins. The variable permeability and diverse exchange mechanisms of hyporheic zones result in heterogeneous conditions, posing a significant challenge for modeling coupled physical and biogeochemical processes. Studies often focus on individual aspects (e.g., physical, chemical, biological) of hyporheic zone dynamics due to data constraints, limiting comprehensive understanding and scaling efforts. The team took a hypothesis-driven approach that integrates theoretical knowledge generation, model development and experimentation to address this challenge. Starting with conceptual models built from known theory and data patterns, researchers identified key hypotheses that were testable with available data. Using a continental-scale dataset from the Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS) consortium, researchers first tested the prediction that sediment respiration rates would decrease as the number of unique organic molecules (i.e., OM molecular richness) increases. The analyses rejected the hypothesis of a direct limitation of respiration by OM molecular richness. Rather, the team found that OM concentration and thermodynamics impose primary constraints on sediment respiration. Researchers further conducted numerical experiments to explore the potential controls using a simple thermodynamic-based kinetic model, where OM thermodynamics, microbial biomass and substrate accessibility were included as key drivers.

Integrating numerical experiments and observational data, it was determined that the OM molecules fueling respiration comprised less than 1% of the measured OM. These results motivate deeper evaluation of the physical characteristics of river sediments that modulate the physical accessibility of OM, such as particle size, specific surface area and density of surface binding sites. The hypothesis-driven approach is a powerful way of integrating models and observations. The continental-scale WHONDRS dataset allowed researchers to challenge and refine existing hypotheses with numerical experiments, and to build geographically transferable predictive models and deeper, process-informed understanding.

#### Watershed Dynamics and Evolution Science Focus Area

#### Watershed Dynamics and Evolution Science Focus Area: Overview

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#### https://wade.ornl.gov

The freshwater provisioning and regulating services provided by mid-order watersheds are under increasing stress driven by accelerating changes in land use and land cover (LULC) and an intensifying hydrologic cycle. Predicting the long-term consequences of such hydrologic intensification and LULC change (watershed evolution) at regional scales requires an improved, transferable understanding of how watershed function depends on environmental conditions (watershed dynamics). The Watershed Dynamics and Evolution (WaDE) science focus area project aims to advance predictive understanding of how dominant processes controlling watershed hydro-biogeochemical function operate under a range of hydrologic regimes and vary along stream networks that drain heterogeneous land covers.

The WaDE research plan addresses critical knowledge gaps related to how watershed function responds to exogenous change, using stream metabolism as a key integrative measure of upland-stream interactions and stream corridor processes. The team also address gaps in observation networks that have been biased toward higher-order streams with homogeneous watershed LULC by systematically targeting watersheds with heterogeneous land cover that are broadly representative of watersheds in the Tennessee River Basin (TRB), the most intensively used freshwater resource region in the contiguous United States.

In this presentation the team will discuss progress made towards fulfilling overarching goals. Since June 2023, the team has not only published manuscripts, but researchers have held the annual all-hands meeting, performed storm sampling during the first flush after an unprecedented drought, encoded a representation of stream metabolism in the Advance Terrestrial Simulator tool, engaged in science, technology, engineering, and mathematics (STEM) outreach discussions with Oak Ridge High School (TN), selected and instrumented all of the intensive sites in watershed 1 (East Fork Poplar Creek, TN), initiated observations in watershed 2 (Reddy Creek, TN), and have placed sensors in 24 other mid-order watersheds across the TRB to evaluate watershed similarity assumptions.

#### Watershed Dynamics and Evolution Science Focus Area Theme 1: Dynamic Headwaters

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#### https://wade.ornl.gov

Non-perennial streams that periodically cease to flow constitute a large portion of global stream networks; however, their contributions to watershed function and downstream hydro-biogeochemistry remain unclear. Theme 1 in the Watershed Dynamics and Evolution (WaDE) science focus area evaluates the ecohydrology, biogeochemistry, and microbiology of nonperennial streams (dynamic headwaters). The team characterizes processes that control the quantity and composition of water and solutes that are transported from upland catchments into the stream network. The goal is to understand how variable streambed saturation drives hydro-biogeochemical processes that influence downstream metabolism. Here, researchers examine flow patterns and concentrations of carbon species, other nutrients, and trace metals in non-perennial tributaries across different types of land cover to evaluate contributions from weathering and potential anthropogenic sources. Data obtained on the frequency and duration of flow in nonperennial streams will be used to improve representation of nonperennial streams in watershed-scale models. Researchers are also intensively monitoring two nonperennial streams draining contrasting urban and forested areas to study how surface-groundwater interactions, plant water use, redox biogeochemistry, and microbial communities respond to variable flow. The redox-sensitive metals iron and manganese are known to regulate the solubility, transport, and transformation of organic matter and micronutrients, such as trace metals. Under no-flow conditions, iron and manganese metal precipitates can accumulate in disconnected pools along the stream channel. During high-discharge events,

the mobilization of particles and colloids may contribute significantly to the export of nutrients and trace metals from uplands. The field and laboratory studies performed will resolve how colloid and particle dynamics influence (micro) nutrient levels across saturation and redox gradients generated through intermittent flow.

#### Watershed Dynamics and Evolution Science Focus Area Theme 2: Stream Corridor Processes

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https://wade.ornl.gov

Theme 2 of the Watershed Dynamics and Evolution (WaDE) science focus area characterizes stream corridor processes at the reach scale using a combination of field experiments, laboratory mesocosm studies, and modeling. Mid-order streams are reactive conveyors that receive, process, and transport carbon, nutrients, and other solutes from upstream and the surrounding uplands. Nevertheless, they are noticeably underrepresented in the research literature so quantitative understanding of their roles in watershed function is lacking. Specific questions and hypotheses address (1) Quantifying the contributions of water column gross primary production (GPP) and ecosystem respiration (ER) to net ecosystem production (NEP) across gradients in land cover, (2) Elucidating the effects of organic matter burial in the stream benthos on aerobic versus anaerobic metabolism, and (3) Assessing the resistance and resilience of reach-scale GPP and ER to disruption by transient high flow events.

The team has established three long-term observation stations that span dominant land-cover categories within the first research watershed. Using a combination of manual sampling across a range of flow conditions and continuous water quality data collected with multiparameter sondes, researchers are analyzing element and nutrient yield across the watershed. When normalized to sub-watershed area, DOC flux is comparable among sites with marginal seasonal differences. Concentration versus discharge curves suggest allochthonous sources of organic carbon enter the stream during rain-driven floods. Nutrient spiraling analysis shows uptake lengths for nitrate, ammonium, and phosphate are long (on the order of kilometers), consistent with chronically high nutrient concentrations characteristic of urban-influenced streams. Overall, there is net removal of nitrate and phosphate and net release of ammonium. Initial estimates of dissimilarity among sites using the multivariate time series indicate (1) dissimilarity changes with time in response to watershed-wide controls, and (2) in periods of

constant dissimilarity, the contribution of individual variables to dissimilarity estimates changes with time.

#### Watershed Dynamics and Evolution Science Focus Area Theme 3: Organizational Controls on Stream Function Within and Across Mid-Order Watersheds with Heterogeneous Land Cover

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#### https://wade.ornl.gov

Anthropogenic activities are altering watershed hydrology and land use-land cover with cascading effects on the storage, processing, and transport of water, nutrients, carbon, sediments, metals, and contaminants from watersheds. Theme 3 of ORNL's Watershed Dynamics and Evolution (WaDE) science focus area seeks to resolve the large-scale organizational controls on emergent patterns and regimes in stream function (especially stream metabolism) within and across mid-orders stream networks with heterogeneous land cover. This presentation will provide an overview of resultsto-date focused on evaluating the spatiotemporal controls on network-scale synchrony/asynchrony in stream metabolism and related metrics of watershed function. Building upon earlier site-selection efforts, the team instrumented 25 mid-order watersheds within the upper and middle Tennessee River Basin (TRB) selected to be representative of extant variation within the TRB based on previous cluster analysis. High-frequency *in situ* sensors were installed at the outlet of each watershed in March 2023, before leaf out, to track the response in flow, temperature, specific conductivity, and dissolved oxygen (DO) over time and across systems. Researchers are using this data to test the high-level hypothesis that patterns in watershed function can be predicted by key state and forcing variables. At the first intensive watershed, East Fork Poplar Creek (EFPC), researchers have been collecting a series of measurements at 14 core sites across the stream network, including high-frequency DO, temperature, conductivity, and depth timeseries; monthly water chemistry and discharge (often coinciding with Theme 1 and/or Theme 2 sampling campaigns); and bi-monthly measurements of organic-matter decomposition using cotton strips. This EFPC data is being used to evaluate synchrony/asynchrony in metabolic processes and drivers across the stream network.

#### Watershed Dynamics and Evolution Science Focus Area Modeling Crosscut: Modeling the Effects of Hyporheic Zone Processes on Stream Oxygen Dynamics

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#### https://wade.ornl.gov

The Modeling Crosscut Activity of the Watershed Dynamics and Evolution Science (WaDE) science focus area is developing a virtual watershed capability focused on watershed hydrology, water temperature, and stream metabolism. This capability supports WaDE's research themes and is critical for efforts to gain a transferable understanding of hydrobiogeochemical regimes in watersheds with heterogeneous land covers.

The team summarizes its ongoing efforts to improve understanding of whole-stream metabolism and its conceptual representation for modeling and data interpretation. Specifically, researchers use a new multiscale model for reactive transport in stream corridors to investigate how hyporheic exchange flows and heterotrophic respiration in the hyporheic zone interact to influence oxygen dynamics in stream channels. The multiscale model associates a subgrid model for hyporheic transport and reactions with each computational grid cell in a channel network model. The approach differs from the classical transient storage model in that it represents a diversity of advective flowpaths characterized by the hyporheic travel time distribution. Researchers configure the multiscale reactive transport capability in the ATS code to represent the key processes controlling oxygen dynamics: (1) gross primary production (GPP) and respiration (Rc) in the channel, (2) oxygen exchange with the atmosphere, (3)hyporheic exchange and advective transport, and (4) aerobic respiration (Rs) in the hyporheic zone. Rs kinetics are represented as a dual Monod process. Researchers use this conceptualization to identify dimensionless parameters that collectively control oxygen dynamics.

Researchers then performed a meta-analysis of publicly available datasets across the conterminous United States to constrain the variability of these dimensionless quantities in natural systems. Finally, the new model and the meta-analysis results were used to perform a detailed global sensitivity analysis and Bayesian inverse modeling to assess potential biases arising from neglecting mass transfer limitations, as is commonly done in the single-station method for estimating GPP and ER from time-resolved oxygen measurements.

#### Watershed Function Science Focus Area

#### The Impact of Disturbances on the Trait-to-Function Relationships Underpinning Watershed Biogeochemical Cycling

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#### https://watershed.lbl.gov

Mountainous watersheds are characterized by strong gradients in functional traits, including vegetation, topography, geology, and geomorphology, which together determine nitrogen (N) retention, and release. Uncertainty remains as to how atmospheric warming within mountainous regions, which increases water limitation and the severity of drought, will impact trait-to-function relationships underpinning the N cycle. This contribution details recent and upcoming work examining, through integrated measurements, manipulations, and modeling, how disturbance in subalpine ecosystems uncouples trait-function relationships and feeds back on biogeochemical cycling. Researchers start by addressing how distinct watershed traits dictate the retention and release of N, by characterizing the N cycle in paired catchments within the East River watershed. The East River catchment, underlain by N-rich Mancos shale with a mixed land cover, exported ~3.5 times more nitrate than the conifer-dominated Coal Creek. The conservative N-cycle within Coal Creek is likely due to the abundance of conifer trees, and smaller riparian region, retaining more NO<sub>3</sub>- overall. The East River shows evidence of stronger biogeochemical cycling of N, where the aggregate export signal is regulated by physical and biogenic processes. To improve the characterization of the East River N cycle over time, researchers built a simple model of the terrestrial-aquatic N cycle predicated upon the most critical traits identified previously. Subsurface water residence times, which dictate transport or reactivity, are determined by coupling the model to Par-Flow-CLM. Here, through a series of atmospheric warming experiments, researchers address how disturbance alters trait-to-function relationships, and subsequently N export. Researchers note that warming reduces hydrologic connectivity and impedes assimilation and transformation of N by plants and microbes. As such, exports of N from the East

River catchment are predicted to decline under future climate conditions. However, distributions of traits (e.g., vegetation, microbial) are not static and more dynamic modeling approaches may be necessary to capture system adaptation to future climate conditions. Finally, in addition to pervasive water limitation, biogeochemical cycling can also be impacted by acute trait redistribution following pulse disturbance (e.g., wildfire, beetle outbreaks), or management (e.g., thinning, clear cutting) to coupled hydrological, ecological and biogeochemical processes. Researchers outline the plans to leverage proposed adaptative forest management activities within Trail Creek to address questions concerning how hydrologic connectivity and biogeochemical cycling change following abrupt shifts in trait distribution, and the consequences for downslope forest community resilience to drought, and biogeochemical cycling in riparian regions.

#### Advancing Watershed Science Via Multiscale Data and Model-Experiment (ModEx) Integration

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https://watershed.lbl.gov

Implementing an integrated model-experiment (ModEx) approach in watershed science necessitates a robust framework for multi-scale data collection, management, and datamodel integration. This comprehensive approach is pivotal in fostering a synergistic relationship between experimental observations and model simulations, enhancing the understanding of watershed dynamics and functions. At East River, researchers collect and utilize multiple observations, including remote sensing, in-field sensing and sampling, and laboratory analysis. A framework that integrates these data for calibrating and validating watershed models is central to the ModEx approach. Specifically, researchers have leveraged decadal-scale remote sensing datasets to unravel complex vegetation dynamics within the watershed. This analysis provides insights into the correlations and potential impacts on vegetation from key watershed traits, including

topography, bedrock composition, and their interactions with changing climate. Additionally, the extensive network of in-field sensors, crucial for real-time data collection, monitors parameters like soil moisture, temperature, and wind speed, providing detailed datasets that capture the dynamic nature of the watershed environment. For the next phase, researchers aim to enhance ModEx framework integration by acquiring new observations through a model-guided approach for sample collection and sensor deployment. The data-gathering campaigns will feed into developing and applying ATS-EcoSIM, the core hydro-biogeochemical simulation capability. ATS-EcoSIM development will feature a dynamic, trait-based model of plant-soil-microbial interactions to understand emergent behaviors in response to interacting press and pulse disturbances. The Science Focus Area (SFA) data management and integration component offers infrastructure and services for the project's data lifecycle, including data publication, wireless sensor connectivity, automated quality checks of sensor datasets, and integration of diverse time-series data for analysis and modeling. The ModEx approach, developed in the SFA, offers transferable, validated methodologies to the broader scientific community, enhancing collaboration, data sharing, and cross-disciplinary integration, and ensures that the data management, observation, and modeling insights are applicable in wider research contexts.

#### Student

#### Scaling of Watershed Functional Trait Co-Variability

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Key to understanding watershed functions is characterizing aboveground (e.g., vegetation dynamics, topography) and belowground (e.g., soil and bedrock structures) properties, which in turn govern patterns of important hydrobiogeochemical processes. These important properties are defined as watershed functional traits: properties whose coevolution and resulting covariance and interactions regulate the behavior of a watershed. However, it is challenging to capture these traits on the watershed scale, often due to their high heterogeneity. Partitioning watersheds into a series of hillslopes offers both the opportunity to narrow these heterogeneities and to examine co-variability across above- and belowground traits. The team utilized two adjacent Colorado watersheds, the East River and Taylor River, which display a diverse set of bedrock-through-canopy characteristics, such as geology, vegetation coverage, and snow coverage. Using topography, researchers delineated watersheds into appropriate hillslope units based on multiple threshold drainage areas and determined key hillslope metrics from geospatial layers.

Specifically, the team investigated the relationship between plant species distribution, subsurface structure, and hillslope geometry. By varying threshold drainage area, researchers investigated the scaling relationships between hillslope size, trait co-variability, and the ability to capture watershed-wide variability in these metrics. Results showed that across both watersheds, hillslope-averages of slope and elevation are significantly correlated and that conifer-dominated hillslopes are primarily located in mid-slope, mid-elevation, and granitic rock regions. The diversity of geology in the East River watershed might be associated with mixed vegetation types.

#### Relationships Between Watershed Scale Co-Variability of Traits and Watershed C-Q Function

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#### watershed.lbl.gov

Predictions of stream hydro-biogeochemistry including chemistry and discharge (C-Q) in response to hydrological perturbations involve physically based models. Spatially distributed models rely on the availability of geospatial trait data layers, which are difficult to obtain at spatial-temporal scales compatible with model grid sizes. These data layers are often created from limited spatial data and statistical models to extrapolate/interpolate spatially. To overcome these inherent limitations, new approaches have been proposed to harness the remote sensing spatial covariates to predict other parameters such as soil hydraulic conductivity, soil geochemical properties, and bedrock properties. Additionally, characteristic and reproducible C-Q patterns emerge at different scales, and these C-Q patterns contain information on hydrological, ecological, and biogeochemical dynamics within a watershed, yet these patterns and associations between co-variability of traits and C-Q as a watershed function are not well understood.

The watershed study leverages in-stream data as aggregated observations of C-Q watershed response to changing snow conditions to advance understanding of watershed function in response to trait co-variability. Researchers investigate the >30 year record of historical C-Q data available for the East and Taylor River watersheds. Researchers have chosen to use watershed C-Q relationships because hydrologic connectivity, and ecological and hydro-biogeochemical processes vary in space and time, such that dynamic C-Q relationships, measured within and between watersheds, may be diagnostic of how watershed functional traits are interacting and changing.

Researchers extend the prior developed zonation approach and evaluate the co-variability of traits by applying clustering to multiple data layers. A particular focus is to explore the transferability of the zonation approach to different basins as well as to investigate the impact of spatial resolutions and scales. Using spatially resolved maps of traits, and field observations of C-Q collected since 2014 (Upper East) and since 1970 (larger East and Taylor), including export of nitrogen and other elements at multiple locations within the both watersheds, researchers explore C-Q response variability across elevations, the relationship with dynamic traits (vegetation, microbial), and more static traits (bedrock, topography). Trait importance to C-Q outcomes is explored using sensitivity analyses with trait-informed numerical models in a one-factor-at-a-time approach.

### Toward the Understanding of Biogeochemical Functions of the Future Floodplain

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Floodplains act as critical buffer zones between mountain hillslopes and rivers, regulating water and element (e.g., nutrients, colloids) exports to rivers. Concurrent temperature changes and increased hydrologic pulse disturbances will change the function of floodplains in the future. As floodplains physically and biologically rearrange in response to these drivers, there will be concomitant changes in floodplain hydrologic partitioning and biogeochemical functioning. Yet, the consequences of interacting hydrological and ecological impacts of disturbances on element retention capacity of future floodplains are still unknown.

The hydrologic connectivity between hillslopes, floodplains, and rivers drives biogeochemical processes and exchange fluxes. Through a series of lab, field, and modeling experiments, the team recently demonstrated that disturbances in hydrologic connectivity and water chemistry impacted floodplain biogeochemical processes in previously unpredicted ways; fine-scale sediment heterogeneities and colloidal transport had orders of magnitude larger impacts than what was predicted by "traditional" modeling/theory. Furthermore, modeling and field observations suggest that hydrologic regime changes will drive changes in vegetation (e.g., grasses replacing willows) of future floodplains with implications for water/nutrient retention capacity. For example, DNRA tends to decrease in absence of willows, likely leading to increased nitrification and decreased nitrate retention.

Researchers expect future natural and managed adaptations (e.g., beaver dams, forest management) to mitigate the impacts of hydrological dynamic changes. The recent studies show that beaver dams overshadow climatic hydrologic extremes in their effects on water residence time and nitrogen fluxes in riparian zones.

Going forward, the team will instrument and sample floodplains that exhibit recent hydrological and vegetation changes corresponding to various scenarios predicted for a future climate and planned management experiments (e.g., beaver dam analogs, forest management). These test sets will help researchers understand the changes that can be expected in the future and prepare useful and actionable predictions of future floodplain functioning.

#### Exploring the Role of Subsurface Traits on Subalpine Ecosystem Response from Seasonal to Decadal Time Scales

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The response of subalpine ecosystems to varying water availability has important implications for the retention and export of carbon (C), nitrogen (N), and water. Researchers investigate how the dominant subsurface characteristics (traits) play a critical role in forest's drought response. This research question is addressed by using an iterative modelexperiment (ModEx) approach based on observations of ecosystem response dynamics from seasonal to decadal time scales to benchmark simulations of the C, N, and water stores and fluxes along a 2D transect with the mechanistic ecosystem model ecosys. The study site is an intensely instrumented hillslope on Snodgrass mountain in the East River Watershed. The ecosys simulations provide insights into site characteristics ("functional traits") that determine the ecosystem fluxes ("function"). Based on the modeling results researchers further identify necessary observations to improve model fidelity. The model benchmarking data include decadal observations that show how climatic drivers impact differently on granodiorite and shale bedrock, tree ring growth, and element concentrations (e.g., Ca, P, Sr via XRF imaging) in Lodgepole pine and Engelmann spruce tree cores. Remotely sensed variations of the Normalized Difference Vegetation Index based on Landsat images, allows relating the tree ring data to forest health dynamics along Snodgrass mountain. Researchers further use time-lapse electrical resistivity tomography (ERT) measurements along the modeling transect to understand the contrasting water storage and flux dynamics in shallow soils beneath the conifer forest canopy upslope and deep colluvium soils beneath meadow vegetation downslope. Nine ERT transects in combination with terrestrial Light Detection and Ranging (LiDAR) scans of the forest stand structure further highlight the relation between soil and bedrock traits and ecosystem function (i.e., biomass) that informs the ecosys model structure and parameterization. Regular sampling of suction lysimeters and resin samplers provide dissolved element concentrations (e.g., nitrate) and snapshot sampling campaigns showed the C and N stocks across soil profiles and in the conifer leaves.

Stable isotopes of water in soils and tree xylem identify the tree's dominant water source on Snodgrass mountain. Based on the outlined combination of aboveground and below-ground observations providing information of ecosystem response from inter-annual to decadal time scales, researchers improve the mechanistic representation of the climate driven interactions between vegetation and subsurface traits in the *ecosys* model. Researchers highlight how feedbacks due to these interactions play out during exceptionally wet periods (e.g., 1995) and extremely dry years (e.g., 2010), which prepares researchers to assess ecosystem response to future climate scenarios.

#### Colloid Generation, Stability, and Transport in Redox-Dynamic Mountain Watersheds and Impact on Water Quality in Alluvial Sediments

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Mountainous watersheds are experiencing more frequent interacting press and pulse disturbances that create new hydrological regimes with consequences for biogeochemical transformations at critical interfaces. For example, episodic wet-dry cycling at solid-water interfaces promote shifts in aqueous phase parameters (pH, oxygen, ionic strength, and ionic composition) and chemical, organic and mineral transformation of the solid phase, generating colloids (1 nm to 1 μm), and/or influencing colloidal stability. Being typically associated with organic matter, micronutrients, and contaminants, colloids may serve as transport vectors throughout redox-affected terrestrial and aquatic systems, impacting biogeochemical reactivity downstream and the products exported to ground-/surface waters. Despite evidence that redox cycles play a significant role in generation and transport of colloids, the mechanisms, chemical composition, reactivity, and stability of generated colloids are poorly understood.

To resolve this knowledge gap, researchers developed an approach to detect physico-chemical composition of different particles using Asymmetric Field Flow Fractionation combined with ICP-MS, UV-, fluorescence-, MALS- and zetasizer-DLS detectors. Separation of colloids and collection in redox- preserved conditions then enables deeper molecular-scale characterization (e.g., TEM, STXM, XAS, NanoSIMS). Previously, researchers have examined the impact of redox changes on the generation and transport of colloids through a transect from bedrock to floodplains through a series of laboratory and field experiments. This work revealed that oxidative dissolution of pyrite from bedrock at neutral pH generates 50 to 100 nm Fe-colloids, promoting the mobilization of nutrients and contaminants (e.g., Ni and Cr). In floodplains, these results show that low sulfidation increases colloid stability of ferrihydrite, whereas higher sulfidation (S/Fe<0.5) generates nano-scale FeS colloids. In natural samples, ferrihydrite colloids remained stable under sulfidic conditions, which could be due to the passivation by organics as the team confirmed through lab-simulations. Finally, incorporating colloidal transport highlighted in the column experiments significantly improved accuracy of model predicting floodplain biogeochemical processes.

#### Model-Based Interpretation of Hydrological and Biogeochemical Functional Traits of Hillslopes in a Mountainous Watershed

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Declining snowpack, modification of precipitation patterns, and increasing temperature are rapidly altering the quantity and quality of water exported from headwaters. Hillslopes represent dominant landforms of mountainous watersheds and therefore exert fundamental controls on hydrological cycles and chemical composition of floodplains and rivers. However, subsurface processes controlling water partitioning and solute exports on mountain hillslopes remain poorly understood due to the heterogeneity of watershed traits characterizing the Critical Zone (e.g., bedrock lithology, topography, vegetation cover) and the impacts of local climatic conditions. This knowledge gap limits the ability to predict the evolution of high elevation watersheds experiencing climate change. Physics-based models are powerful tools to mechanistically unravel subsurface hydro-biogeochemical functioning and are key for the quantitative understanding of the traits that modulate water flow and solute exports.

In this study, researchers implement a new generation of HPC-enabled numerical models (e.g., ATS, CrunchFlow, PFLOTRAN) capable of simulating hydro-biogeochemical fluxes from hillslopes at seasonal timescales. Based on a comprehensive dataset characterizing: (1) the subsurface physico-chemical properties (e.g., geophysical measurements of bedrock resistivity); (2) the vegetation cover; and (3) the local weather conditions, a 3D hydrologic model and a 2D reactive transport model (RTM) are developed at two well-instrumented hillslopes of the East River watershed: Snodgrass and the Pumphouse transect, respectively. The models simulate the temporal fluctuations in partially saturated flow and the transient response of biogeochemical processes to climate events. In particular, for the first time, the 2D reactive transport model explicitly accounts for the connection between soil biological processes and rock weathering as well as multiphase exchange with the atmosphere. These results show the capability of the models to reproduce the dynamic change in snowpack, water content, groundwater table, soil respiration, and fluid chemistry monitored at multiple spatial locations. The calibrated models are used to quantify the relative contribution of shallow versus deep groundwater flow paths characterized by different residence times and biogeochemical conditions in shaping the solute fluxes from hillslopes. Furthermore, researchers perform sensitivity analysis to identify and quantify key functional traits controlling hydro-biogeochemical processes.

The identified functional traits will support the selection of new experimental hillslopes in the Taylor River basin using iterative model-experiment (ModEx) approaches and inform the scaling-up efforts. Finally, the implemented physics-based models will be used to explore the evolution of water flow and solute exports under different future climate scenarios for hillslopes with distinctive traits.

#### Progress in Ecohydrological Model Development for Trait-Based Watershed Modeling

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High-fidelity mechanistic models play a crucial role in comprehending the interplay of ecosystem hydrologic and

biogeochemical cycles, and traits that govern the retention and release of elements in mountainous watersheds. To accurately represent the coupling between hydrological, ecological, biogeochemical, and land-surface processes, adaptive-resolution physics-based models are necessary to capture trait interactions and watershed functions. While various modeling codes capture some aspects to quantify trait interactions and watershed function, none can fully address the entire problem.

The project aims to couple the Advanced Terrestrial Simulator (ATS) with the plant-soil-microbe interactions code EcoSIM. In the proposed coupling, ATS provides water balance and solute transport, while EcoSIM simulates plant water uptake, surface energy balance, microbial dynamics and ecosystem biogeochemistry. The coupling framework follows the established Alquimia library, which was successfully used to add geochemical capabilities to ATS. Specific issues related to ecohydrological processes and EcoSIM require large-volume data transfer and a soil column-based coupling rather than a cell-by-cell one.

Here, researchers present results from baseline hydrological simulations for the East River watershed, CO. Researchers also describe EcoSIM, which is newly developed from its predecessor code ecosys, and provide an update on the ATS-EcoSIM coupling. This update discusses how these combined capabilities will enable researchers to quantify 3D landscape trait interactions and watershed function in the Watershed Function Science Focus Area. East River hydrological simulations show how high-resolution models, parameterized using spatially heterogeneous datasets, can provide a quantitative evaluation of the connection between traits and function, and uncover limitations in the current simplified treatment of land surface processes. Example, EcoSIM simulations demonstrate its capability to simulate typical ecosystems, including forests, grasslands, and wetlands. Test simulations for ATS-EcoSIM demonstrate the development approach, which involves implementing and testing processes separately, starting with surface energy and water, then snow physics, and continuing with plant and microbe dynamics.

#### Mountainous Groundwater Response to Warming and Low-To-No Snow Conditions

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Groundwater is among the least understood components of the coupled hydrologic and biogeochemical cycles in mountainous watersheds, requiring further insights into its dynamics, connectivity to surface water, and watershed traits. To evaluate the effectiveness of groundwater storage in buffering streamflow and evapotranspiration during press and pulse disturbances (such as projections of low-to-no snow years in the coming decades), researchers develop integrated hydrologic models of the East River watershed that couple groundwater with surface water and energy fluxes. Researchers compare model predictions with *in situ* groundwater level and environmental age tracer observations.

At a lower montane hillslope, a high-resolution ParFlow-CLM hydrologic model and EcoSLIM particle tracking model suggest groundwater flowpaths contribute >60% of the water mass flux to the hillslope floodplain. These groundwater flowpaths persist all year and are characterized by decadal to century-scale water ages, which are consistent with mean ages from observed environmental tracers. Extending the particle tracking technique to account for matrix diffusion due to high fractured bedrock traits improves predictions of mixing between young and old-aged groundwater environmental tracers (<sup>3</sup>H and <sup>4</sup>He, respectively). The hillslope models that best match observed <sup>3</sup>H and <sup>4</sup>He suggest groundwater storage has declined over the past decade. This result is consistent with observed groundwater level declines of >1 m since 2016 and potentially highlights the importance of old-aged groundwater storage in streamflow generation. To further interrogate connections between groundwater storage losses and streamflow generation researchers develop watershed-scale 3-D integrated hydrologic models. Simulations show annual runoff efficiency is inversely correlated with groundwater storage efficiency (ratio of annual groundwater storage change to precipitation), suggesting groundwater storage losses buffer runoff efficiencies during low precipitation years. This hypothesis is supported by a majority of simulated groundwater fluxes to streams consistently having water ages >1 year. In a warmer climate, modeling suggests increased forest water use reduces groundwater recharge and results in groundwater storage loss. Losses are most severe during dry years and do

not recover to historical levels during wet periods. Groundwater depletion will significantly reduce annual streamflow and force the basin toward intermittent conditions when precipitation is low. Expanding results across the region suggests groundwater decline will be highest in the Colorado Headwater and Gunnison basins. Ongoing work to validate model predictions with diverse observation datasets will continue to shed light on the role of groundwater on integrated hydrologic processes in mountain systems experiencing changing snowpack conditions.

#### Sensitivity of Groundwater and Surface Water Connectivity to Historical Press and Pulse Climate Disturbances in a Mountainous Watershed

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Groundwater release has the potential to buffer streamflow to short-term climate extremes, but its interactions with surface water in response to climate is largely unknown in mountainous systems with complex terrain. Interactions between climate, snow dynamics, soil water storage, vegetation water use and their effects on groundwater recharge as well as geologic traits influencing storage and transmissivity can affect groundwater contributions to streams. The objective is to assess the importance of groundwater on streamflow in the East River, a Colorado River headwater basin. First, researchers quantify water budget components using an integrated hydrologic model parameterized and validated with extensive data. Model results indicate lateral subsurface flow is a critical mechanism moving snowmelt downgradient to support streamflow, evapotranspiration and to maintain groundwater levels in water-limited portions of the basin. Simulated low-order streams tend toward non-perennial conditions and generate seepage recharge. Higher-order streams occur along valley bottoms and are perennial. They aggregate streamflow from upland portions of the East River and tend toward net groundwater gaining conditions. At the basin-scale, groundwater is found to be an important and stable source  $(26\pm7\%)$  of stream water and directly sensitive to groundwater storage. Groundwater storage aggregates climate over a 4-year period in the East River. Historically, this multi-year aggregation has helped to buffer dry water years and promote groundwater recovery back to the historical

mean condition. Recently, however, the onset of low/no monsoon rain from 2016 to 2020 combined with the shock of an extremely dry water year in 2018 has prompted sustained declines in simulated groundwater storage with average annual groundwater storage losses simulated at greater than 2-standard deviations of the historical mean. This is an example of overlapping pulse events on top of press warming. This agrees with groundwater observations in the East River that indicate hillslope water table declines as a consequence of 2018 are not recovering despite above average snow accumulation in 2019 and 2022. Results from paired air-stream temperature analyses at different locations in the East River will be compared with recession-based analysis, hydrologic model results as well as isotopes and geochemical weathering byproducts to assess spatial and temporal influences of groundwater-surface water exchanges. This will inform future sensor deployment across transects of loworder streams to identify zones of groundwater discharge as a function of catchment traits, constrain integrated hydrological model results, and inform trait-streamflow relationships. Future work will identify watershed traits controlling groundwater discharge zones, variation of groundwater contributions and non-perennial stream extent with climate disturbance across locations with different watershed traits.

#### Modeling the Impact of Engineered Ponding on Floodplain Hydrologic Flow Paths and Solute Transport

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In mountainous watersheds, warmer temperatures and less snow reduce river and groundwater flow. Meanwhile, growing beaver populations help mitigate these effects by enhancing seasonal floodplain storage and possibly groundwater baseflow. Understanding how hydrologic flows change as a function of beaver dams, together with floodplain structures and weather forcings, becomes important for future hydrologic predictions and understanding biogeochemical cycles in various floodplains. Specifically, the transient variations of beaver ponds might induce rapid shifts in redox conditions and subsequently influence the transport of solutes to river and aquifers. However, these impacts of biogeochemical variations from beaver ponds remain poorly understood, particularly in the context of uncertain floodplain structures and weather forcings.

To address this knowledge gap, the team assessed the impact of beaver ponds on hydrological connectivity and thereby the biogeochemical processes in mountainous floodplains, to date focusing on a floodplain along the Slate River, CO. Researchers integrated in situ water level and water quality data, geophysical surveys, and hydrologic modeling, to first reconstruct the hillslope-floodplain structure, and then simulate vertical flow from the topsoil layer to the underlying gravel layer, as well as horizontal groundwater flow. Sensitivity analysis indicated that beaver ponds enhance the cumulative vertical flow, particularly from fine sediment layers to the gravel bed, resulting in an increased export of reduced solutes to the gravel bed. However, beaver ponds have minimal influence on the deeper underflow within the gravel bed aquifer, suggesting that beaver ponds are hydrologically disconnected from deep groundwater flow.

Researchers now plan to employ the same approach to transfer the learned knowledge from the Slate River floodplain to other floodplain structures with varying numbers of beaver dams. For this purpose, researchers will leverage Beaver Dam Analogs constructed by humans to quantify hydro-biogeochemical impacts associated with new beaver dam constructions and compare to floodplains without beaver activity.

#### Wetland Hydrobiogeochemistry Science Focus Area

#### Uranium Speciation in the Rhizosphere and Sediment Compartments in a Riparian Wetland

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

Savannah River Site manufactured nuclear fuel and target assemblies between 1954 and 1989, resulting in significant contamination of Tims Branch (a small stream and its associated wetlands) with uranium (U) and co-contaminant metals (Ni, Cr, Zn, Pb). The Argonne Science Focus Area (SFA; *Wetland Hydrobiogeochemistry*) focuses on understanding the molecular-scale processes that control elemental dynamics in complex environments, such as adsorption, precipitation, and redox transformations. Researchers examined the behavior of contaminant U in the rhizosphere (Kaplan et al. In revision), a region of high reactivity in the sediment near the roots of plants, where visible iron oxides form due to Fe(II) oxidation. U and Fe were found to be significantly more concentrated in the rhizosphere (R) samples compared to the non-rhizosphere (NR) controls. Fe K-edge EXAFS spectroscopy determined goethite and ferrihydrite as the dominant forms of Fe, with the latter present in greater proportions in the R than in the NR samples. U L<sub>III</sub>-edge EXAFS spectroscopy showed U present as U(VI) bound to organic ligands and iron oxides in both the R and NR samples; however, a larger contribution of U(VI) bound to iron oxides was determined in the spectra of the R samples. These results are part of a broader effort by the Argonne SFA to understand U speciation and mobility at Tims Branch, in which approximately 30 cores were collected from the field and analyzed with depth using U L<sub>III</sub>-edge EXAFS spectroscopy.

Saturated, organic-rich sediments at about 5 to 15 cm depth showed the predominance of non- uraninite U(IV) species, whereas drier, near-surface sediments showed the predominance of U(VI) that was bound to the mineral surfaces and to OM entities in the sediment. These studies highlight the intricate interdependencies between the constituents of contaminated sediments and provide speciation information that is necessary for the inclusion of appropriate reactions in reactive transport models.

Kaplan, D. I. et al. In revision. "Uranium Biogeochemistry in the Rhizosphere of a Riparian Wetland," *Environmental Science & Technology.* 

#### Molecular to Micron-Scale Investigations of Floc and Colloidal Fractions of Wetland Groundwater and Surface Waters

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

The mobility and bioavailability of nutrients and contaminants have a strong effect on wetland ecosystem function and are highly dependent upon their: (1) partitioning between solid and solution phases in environmental media; and (2) atomic scale associations with environmental solids. Abundant orange and reddish-brown flocs have been observed along gaining sections of the Argonne Wetland Hydrobiogeochemistry science focus area (SFA) field site at Tims Branch, where anoxic groundwater containing iron(II) discharges into oxygenated stream water. Flocs contain high levels of iron (Fe) and are effective scavengers of phosphorous (P; 2 to 4 wt%), uranium (U; 32 to 600 ppm), and trace metals. The laboratory microcosm studies of these flocs 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). Analysis of material along the depth profile of a core of accumulated floc material shows a progressive reduction of Fe(III) to Fe(II) and U(VI) to U(IV) with depth, consistent with decreasing redox potential.

In addition to characterizing the molecular to micronscale structure of naturally forming flocs at Tims Branch, researchers have also characterized colloids from groundwaters and surface waters. Researchers used tangential flow filtration approaches to size fractionate colloids from groundwater and stream water, under gaining stream conditions. Researchers used a combination of radiochemistry, inductively coupled plasma atomic emission spectroscopy (ICP-AES), Fe K-edge and U L-edge XAFS, <sup>57</sup>Fe Mössbauer spectroscopy, and scanning and scanning transmission electron microscopy (SEM, STEM) equipped with energy dispersive spectroscopy (EDS) to understand the physical and chemical character of the colloids. Molecular scale results indicated Fe-(hydr)oxide and Fe-OM associations within all colloid size ranges. SEM/EDS results consistently identified U associated with carbon- and Fe-rich colloids. U-XAFS analysis identified monomeric U(VI) species in the colloids. STEM analysis resolved individual and spatially separated U atoms associated with many of the colloid OM formations. These results indicate that the vast majority of U within the surface water and groundwater is not in a purely hydrated form but is associated with colloids. The studies of Fe floc and colloid biogeochemistry in Tims Branch and its potential impact on U speciation and transport expand the understanding of their role in the speciation and cycling of

nutrients and trace elements in wetlands, which in turn can lead to more robust modeling of their behavior in aquatic and terrestrial environments.

#### **IDEAS-Watersheds**

#### IDEAS-Watersheds Phase 2: Accelerating Watershed Science Through a Community-Driven Software Ecosystem

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#### https://ideas-watersheds.github.io

The Interoperable Design of Extreme-scale Application Software—Watersheds (IDEAS-Watersheds) project is designed to enhance and broaden the impact of the existing watershed Science Focus Areas (SFAs) within the ESS program through an agile approach to creating a sustainable and reliable software ecosystem.

This poster highlights the unique structure of the IDEAS-Watersheds (Phase 2) project, which is organized around three research activities and four shared infrastructure activities. To ensure integration of the research activities with the SFAs and facilitate training of early career researchers, the team uses a co-funding model with shared deliverables to establish partnerships. These partnerships increasingly embrace a multiscale perspective of the whole watershed and include the Watershed Function SFA (see Lawrence Berkeley National Laboratory-SLAC poster by Molins et al.), the Watershed Dynamics and Evolution SFA (see Oak Ridge National Laboratory poster by Painter et al.), and the River Corridor SFA (see Pacific Northwest National Laboratory poster by Chen et al.). Each research activity is focused through the design of concrete use cases that both advance scientific understanding as well as contribute transferable capabilities to the software ecosystem.

The shared infrastructure activities provide foundational support for the research activities as well as training and community outreach. The Software Stewards activity will ensure the sustainability of the software ecosystem as a community resource and make it more reliable, accessible, and easier to use. The Land Model Interface Activity addresses the critical need for best practices in model setup and analysis of integrated hydroterrestrial models that couple integrated hydrology and land surface models. An Integrated Hydrology Simulation Infrastructure Activity will continue the development of a national hydrology infrastructure that can accelerate regional simulations and improve modeling workflows across modeling platforms. Finally, the team will continue building a community around the software ecosystem through a Training, Community Building, and Outreach Activity.

#### Developing Integrated Hydro-biogeochemical Modeling from Batch to Watershed Scales

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https://ideas-watersheds.github.io

The Interoperable Design of Extreme-Scale Application Software (IDEAS)-Watersheds project focuses on developing general modeling capabilities and workflows that leverage a community software ecosystem to advance hydrobiogeochemical research in watersheds and river corridors and in turn make these advances available to the broader community. The IDEAS-Watersheds' partnership with the Pacific Northwest National Laboratory River Corridor Science Focus Area aims to understand and quantify processes governing the cumulative effects of hydrologic exchange flows, dissolved organic matter chemistry, microbial activity, and disturbances on river corridor hydro-biogeochemical function from watershed to basin scales. The incorporation of hydrologic complexity and molecular-level characterization such as organic carbon chemistry will greatly improve a watershed hydro-biogeochemical model in capturing distinct water quality signatures across variations in land

use, hydrogeology, climate, and disturbances. The team has developed a modeling pipeline that connects molecular characteristics with biogeochemical models and watershed reactive transport models. The organic carbon chemistry inferred from Fourier-transform ion cyclotron resonance mass spectrometry measurements is used to generate new reaction networks and kinetics, which are subsequently tested in PFLOTRAN in batch settings before being incorporated into Advanced Terrestrial Simulator (ATS)-PFLOTRAN for coupled hydrologic and biogeochemical modeling at the watershed scale. Researchers used this coupled model to study biogeochemical transformations of carbon and nitrogen in a few watersheds across the Yakima River Basin in the Pacific Northwest region of the United States. The biogeochemical hot spots and hot moments within the river corridors were found to be strongly influenced by variations in land use, hydrogeology, climate, and disturbances. This pipeline can be extended to allow the incorporation of other omics datasets (e.g., metatranscripts, metaproteomics, and metabolomics) when they become available. This work is also an example of interoperable model development, where generic interfaces such as Alquimia extend the capabilities available from single codes by bringing the capabilities of other codes in the software ecosystem to bear on each specific application.

#### Advancing Stream Metabolism Modeling Through the IDEAS-Watersheds and Watershed Dynamics and Evolution Science Focus Area Partnership

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The modeling partnership between the Interoperable Design of Extreme-Scale Application Software (IDEAS)-Watersheds project and the Watershed Dynamics and Evolution (WaDE) Science Focus Area (SFA) is developing a virtual watershed capability focused on hydrology, water temperature, and stream metabolism. This capability is critical for WaDE's efforts to gain a transferable understanding of hydro-biogeochemical function of watersheds with heterogeneous land covers. The IDEAS-WaDE partnership is using the Advanced Terrestrial Simulator (ATS) code for flow and transport coupled to PFLOTRAN for biogeochemical reactions. The work uses ATS's unique multiscale configuration for stream corridor reactive transport. Toward the goal of improving inferences about stream metabolism from time-resolved oxygen measurements, the team configured the multiscale reactive transport capability in ATS to represent key processes controlling stream oxygen dynamics, including gross primary production in the stream channel, ecosystem respiration in the hyporheic zone, and oxygen exchange with the atmosphere. Researchers are now using that capability to assess limitations of the widely used single-station method for estimating metabolism from time-resolved oxygen measurements.

The partnership is also developing high-resolution watershed models of East Fork Poplar Creek in Tennessee to support the three science themes in the WaDE SFA. To facilitate that effort, several enhancements have been made to ATS and the workflows that support it. An improved representation of sunlight incident on streams, which is an important control on stream metabolism and temperature, was implemented by extending Watershed Workflow to represent stream shading at high resolution, accounting for stream geometry (width and bank height) and vegetation height. New algorithms to produce high-quality streamaligned computational meshes were also implemented in Watershed Workflow. Related to that, the team developed a new capability in ATS to perform transport simulations on the stream-associated subdomain of a larger watershed flow model, which will enable a range of numerical experiments to help understand the relationship between stream metabolism and the surrounding watershed.

#### IDEAS-Watersheds Activities in Partnership with the Watershed Function Science Focus Area

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#### https://ideas-watersheds.github.io

The team summarizes four activities carried out by the Interoperable Design of Extreme-scale Application Software (IDEAS)-Watersheds project in partnership with the Watershed Function Science Focus Area in support of the development and evaluation of models of coupled processes in mountainous watersheds. The project is particularly interested in the representation of land surface processes, which control exchange fluxes between the atmosphere and subsurface.

(1) Simulations of integrated hydrology in the East River watershed are performed by the Advanced Terrestrial Simulator (ATS) using two different meteorological forcing datasets, PRISM and Daymet. Evapotranspiration (ET) is resolved spatially and temporally by means of the Priestley-Taylor model driven by a dynamic leaf area index. The model performance is then evaluated in its ability to capture measured streamflow, snowpack, groundwater, and ET flux in the three subbasins within the watershed.

- (2) ATS is coupled to the land model EcoSIM to access a more complex plant and microbe process representation while using its advanced water and energy physics capabilities. The coupling is being built off the framework established with Alquimia, which has been successfully used to add geochemistry to ATS; here, it must handle the large volume of data associated with ecosystem modeling.
- (3) Recent coupling of the integrated hydrologic model ParFlow with both the E3SM Land Model and the vegetation demography model Functionally Assembled Terrestrial Ecosystem Simulator allows for the joint simulation of three-dimensional and subsurface flow and dynamic vegetation. Coupled watershed simulations of the East River are used to isolate impacts of topography and resultant lateral flow on ET.
- (4) The gas diffusion capabilities in the reactive transport models PFLOTRAN, CrunchFlow, and ATS are benchmarked. This benchmarking by model intercomparison ensures correct capturing of the gas dynamics across the atmosphere subsurface that ultimately exert a dominant control on the oxidation of organic matter and weathering reactions in the shallow subsurface.

# Watershed Sciences DOE Early Career Projects

#### Drying and Rewetting of Riverbed Sediments Leads to Biogeochemical Cold Moments and Shifts Dissolved Organic Matter Thermodynamics

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Currently, over 60% of the global river network undergoes annual wetting and drying cycles. Variable inundation has been shown to impact biogeochemical processes and dissolved organic matter (DOM) composition in riverbed sediments. Differences in respiration between rewetted and constantly inundated sediments, however, remains undetermined, as well as the factors influencing biogeochemical mechanisms and organic matter transformations in wet and dry cycles. With projected increases in stream and river intermittency due to climate change, it is increasingly important to understand effects of drying on key biogeochemical processes like sediment respiration and DOM composition across diverse river ecosystems. To do this, the project studies the effects of variable inundation across 56 sites in the contiguous United States. Researchers conducted laboratory manipulative experiments with sediments from each site where they were either kept constantly inundated or allowed to air-dry over 21 days while being shaken to maintain aerobic conditions. Both treatments were then fully inundated with saturated riverine water and aerobic respiration rates were measured noninvasively using customized oxygen optodes. Samples were collected for ultrahigh resolution mass spectrometry analysis post respiration measurements. The team investigated the effect of drying on DOM chemistry (e.g., DOM properties, elemental composition, and chemical classes) and thermodynamics (e.g., Gibbs free energy and lambda) and the effects of these changes on respiration rates. Results show that while some sites experience little difference in respiration between rewetted and

inundated sediments, others experience decreased respiration, or cold moments, in rewetted sediments compared to those kept constantly inundated. Additionally, drying sediments resulted in a broad range of influences on DOM thermodynamics, respiration rates, and the link between them.

Understanding the impacts of wetting and drying cycles on sediment respiration and how drying affects DOM chemistry and thermodynamics is essential to generate mechanistic inferences regarding the effects of stream intermittency in global biogeochemical cycles.

#### Data-Driven Modeling Strategies for Predicting Stream Flow and Temperature at Watershed to Continental Scales

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#### https://sites.google.com/lbl.gov/inaiads

Accurate and timely predictions of river flows and water quality at local to regional scales are needed to optimize watershed management strategies under a changing climate with increasing occurrences of extreme events. Since extreme events have unpredictable timing, duration, and spatial extents, assessing their impacts on rivers requires the ability to predict in unmonitored or poorly monitored basins. Classical bottom-up approaches for these predictions involve regionalization of statistical or process-based models built at representative, monitored sites based on different measures of watershed similarity. Recent top-down machine learning (ML) models use large continental-scale datasets and increasingly outperform traditional models for regional predictions. Both approaches depend on the concept of similarity based on catchment traits, which are properties such as topography, geology, land cover, land use, and other human activities. These traits interact and co-evolve with each other and with climate forcings to influence how watersheds function at different scales.

Here, the team presents modeling approaches to improve stream flow and water temperature predictions using various data-driven techniques. Researchers compare a top-down deep learning model against a bottom-up transfer learning approach for >1,400 catchments in the United States and examine the appropriate use of watershed traits for both approaches. The project uses networks, mutual information, and feature importance scores to reduce the redundancy in the trait data and determine the optimal set of traits to model different hydrologic functions. Such selection is independently tested in ML models to verify that the chosen traits enhance their predictive power. Results show that the top-down global ML model outperforms the bottom-up models for most sites. The team also finds that although ML models generally perform better with more data, they benefit from having a diversity of training data rather than strictly larger volumes of data and can suffer from performance degradation with redundant inputs.

# Coastal Systems

Coastal sciences research supported by the Environmental System Science program seeks to address key uncertainties in the fundamental and predictive understanding of integrated coastal environmental systems and to improve their representation in Earth system models.

## Coastal Systems **University Projects**

#### Environmental Drivers of Coastal Wetland Biogeochemical Cycling

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The dynamic nature of the coastal terrestrial-aquatic interface (TAI) means that biogeochemical cycling can be highly variable in responses to continued or episodic changes in environmental drivers. Incorporating the coastal TAI into Earth systems models requires a better mechanistic understanding of the biogeochemical processes that regulate greenhouse gas (GHG) emissions. In response, researchers started a model experiment (ModEx) project in 2021 in which they use automated measurements of wetland GHG emissions combined with mesocosm global change experiments to gain a predictive understanding of the mechanisms controlling anaerobic decomposition and GHG emissions in the coastal TAI so that these processes and their casual factors can be incorporated into process-oriented biogeochemical models.

Researchers have been using autochambers to measure continuous methane (CH<sub>4</sub>) and carbon dioxide (CO<sub>2</sub>) emissions since April 2021 and nitrous oxide (N<sub>2</sub>O) emissions since Nov 2023. In January 2024, the chambers successfully collected data while floodwaters were 95 cm above the soil surface, the third highest flooding event on record. Initially the team observed strong diurnal patterns where CH<sub>4</sub> emissions were lower and more variable during the day than at night, but there was surprisingly no diurnal pattern in 2023. Though soil temperature is a strong driver of the magnitude of CH<sub>4</sub> fluxes, researchers also found that CH<sub>4</sub> emissions are suppressed during high salinity periods. Thus far, N<sub>2</sub>O emissions are highly variable, but overall quite low during winter months.

The mesocosm experiments are designed to understand the biogeochemical mechanisms underlying the field observations, so that they can be incorporated into process models. From June 2022 to October 2023, the team conducted a sea level rise (SLR) experiment using mesocosms with and without vegetation at two salinity levels. Overall, researchers found that SLR increases CH<sub>4</sub> emissions from both brackish and freshwater marshes while warming has a larger impact on CH<sub>4</sub> emissions from brackish marshes. In incubation experiments, methanol was the best source of carbon for CH<sub>4</sub> production across both salinities, followed by methylamine, whereas acetate was only a major substrate for methanogenesis in freshwater wetlands. In June 2024, the team will start a new mesocosm experiment focused on GHG responses to pulses of inundation, salinity, temperature, and nutrient availability.

#### Tidal Triggers and Hot Spot Switches in Coastal Marsh

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Plum Island Estuary is the largest remaining tidal wetland complex in the northeastern United States. During drought in July 2022, eddy covariance revealed a surprisingly rapid switch in ecosystem-scale biogeochemistry of methane in the estuarine oligohaline zone. Methane (CH<sub>4</sub>) flux from *Typha angustifolia* marsh to the atmosphere plummeted from ~200 nmol m-<sup>2</sup> s<sup>-1</sup> to near zero within hours of inundation by an unusually saline tide (Forbrich DE–SC0022108). Reduced CH<sub>4</sub> flux to the atmosphere was sustained for months despite persistent CH<sub>4</sub> pools in sediment porewater. Researchers are testing four hypotheses related to CH<sub>4</sub> production and consumption:

- **Hypothesis 1.** Salinity stress induces increased catalase activity in *Typha* roots, leading to enhanced root O<sub>2</sub> release from the H<sub>2</sub>O<sub>2</sub> produced during stress. Aerobic *methanotrophy* may therefore increase in rhizosphere hot spots of enhanced O<sub>2</sub> availability.
- **Hypothesis 2.** Anaerobic methane (ANME) oxidation in the upper 10 cm (hot layer) of sediment is stimulated by saline inundation. ANME archaea in consortia with sulfate reducing bacteria are potential actors.
- **Hypothesis 3:** Methylotrophic methanogens produce methane despite high porewater sulfate concentration.
- **Hypothesis 4.** *Typha angustifolia* roots produce glycine betaine as a compatible osmolyte, which, once fermented to trimethylamine, could make roots hot spots for support of methylotrophic methanogenesis.

Results of hypothesis testing will guide developments within the E3SM-PFLOTRAN marsh modeling framework. Field-robust planar optode systems were developed and deployed Oct. 2023, revealing remarkably dynamic  $O_2$  concentrations to 15 cm depth with tidal forcing.

**Potential impact:** Incorporation of microbial and plant mechanisms into process-based models has tremendous potential for improving understanding and prediction of  $CH_4$  emissions as coastal terrestrial-aquatic interfaces experience sea level rise and more frequent saline inundation. Evidence is accumulating from diverse ecosystems that methylotrophic methanogenesis can proceed at high salinity.  $H_2O_2$  production and the induction of catalase during stress is widely shared across plant species, suggesting catalase-dependent oxygenation of the rhizosphere could be generalizable.

#### Carbon Dynamics in Response to a Shifting Terrestrial Aquatic Interface in Coastal Plain Wetlandscapes

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Water table variation in low-relief landscapes creates a dynamic terrestrial-aquatic interface (TAI), the ebb and flow of which controls reactions that stabilize or remineralize organic matter. Geomorphic heterogeneity in wetland depressions creates functional variation in water storage and connectivity over space to complement the temporal variation intrinsic to seasonal hydrometeorological forcing. Researchers seek to understand how landscape-scale variation in hydrology and topography, and by extension the shifting position and length of the TAI, regulate the storage and export of carbon (C) via both vertical and lateral pathways. The early work on this project has been to concatenate digital terrain data, existing water level time series in wetlands and streams, and remote sensing of upland and wetland forest productivity to characterize (i.e., model) the extant variation in hydrological conditions in two hydrologically contrasting wetlandscapes in northern Florida. Based on this variation, the team chose 12 wetlands and 10 streams to instrument for continuous and synoptic variation in water level, soil redox conditions, greenhouse gas production rates using low-cost telemetered environmental sensors. Researchers further initiated sampling to explore within-site variation in the quantity and quality of stored organic matter. The objective is to synthesize the hydrotopographic controls on C storage and release from these dynamic landscapes, and embed these functions more realistically in land surface models by structuring subgrid variation to reflect the changing extent of wetland and upland extent with a shifting TAI.

#### 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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This project's goal is to improve mechanistic process understanding and modeling of tidal wetland hydro-biogeochemistry in coastal terrestrial-aquatic interfaces (TAIs). Key characteristics distinguish coastal wetlands, including tidal oscillation, sulfur biogeochemistry, and plant structural adaptations to anaerobic soil. These characteristics have only very recently been incorporated into land surface models such as ELM-PFLOTRAN and 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 flow 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. In 2023, researchers continued to monitor porewater data of nutrients, carbon (C) and methane  $(CH_4)$  and stable isotopes of CH<sub>4</sub> as well as ecosystem-scale flux measurements in a brackish marsh in the Parker River estuary in MA. In July 2023, the research team started to see an increase in CH4 fluxes. This indicates the start of recovery of microbial activity after the sharp drop researchers observed in summer 2022 during a high salinity flooding event. Researchers find that physicochemical variables are the most important predictors for this behavior, more so than C fluxes. Furthermore, researchers have started to experimentally test salinity impacts on CH<sub>4</sub> production and oxidation (Cardon DE-SC0024270). The team also continued with field-testing spatially explicit sediment redox measurements. Researchers successfully captured tidal flooding impacts of belowground oxygen pools in two locations with contrasting hydrology (creekbank and marsh interior). In modeling work, the team has successfully set up different scenarios of root oxygen release in PFLOTRAN. Using these scenarios, researchers have then conducted a sensitivity analysis to assess to which the simulated CH<sub>4</sub> flux responds the strongest. The team plans to transfer this information into ELM-PFLOTRAN.

#### STUDENT

#### Changes in Inundation Drive Carbon Dioxide and Methane Fluxes in a Temperate Wetland

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Wetlands cycle carbon by being net sinks for carbon dioxide  $(CO_2)$  and net sources of methane  $(CH_4)$ . Daily and seasonal temporal patterns, dissolved oxygen (DO) availability, inundation status (flooded, dry, or partially flooded), water depth, and vegetation can affect the magnitude of carbon uptake or emissions, but the extent and interactive effects of these variables on carbon gas fluxes are poorly understood. Researchers characterized the linkages between carbon fluxes and these environmental and temporal drivers at the Old Woman Creek National Estuarine Research Reserve (OWC), OH. The team measured diurnal gas flux patterns in an upstream side channel (called the cove) using chamber measurements at six sites (three vegetated and three nonvegetated). Researchers sampled hourly from 7 a.m. to 7 p.m. and monthly from July to October 2022. DO concentrations and water levels were measured monthly. Water inundation status had the most influential effect on carbon fluxes with flooded conditions supporting higher CH<sub>4</sub> fluxes (0.39 µmol CH<sub>4</sub> m<sup>-2</sup> s<sup>-1</sup>;-1.23 µmol CO<sub>2</sub> m<sup>-2</sup>  $s^{-1}$ ) and drier conditions supporting higher CO<sub>2</sub> fluxes  $(0.03 \,\mu\text{mol}\,\text{CH}_4 \,\text{m}^{-2}\text{s}^{-1}; 0.86 \,\mu\text{mol}\,\text{CO}_2 \,\text{m}^{-2} \,\text{s}^{-1}).$  When flooded, the wetland was a net CO<sub>2</sub> sink; however, it became a source for both  $CH_4$  and  $CO_2$  when water levels were low. Researchers compared chamber-based gas fluxes from the cove in flooded (July) and dry (August) months to fluxes measured with an eddy covariance tower whose footprint covers flooded portions of the wetland. The diurnal pattern of carbon fluxes at the tower did not vary with changing water levels but remained a CO<sub>2</sub> sink and a CH<sub>4</sub> source even when the cove where researchers performed the chamber measurements dried out. These results emphasize the role of inundation status on wetland carbon cycling and highlight the importance of fluctuating hydrologic patterns, especially hydrologic drawdowns, under changing climatic conditions.

Hassett, E., et al. 2024. "Changes in Inundation Drive Carbon Dioxide and Methane Fluxes in a Temperate Wetland," *Science of The Total Environment* **915**, 170089. DOI:10.1016/j.scitotenv.2024.170089.

#### Virtual

#### Mapping Hot Spots of Metabolic Potential in Salt Marsh Sediments with Multiplexed Fluorescence *In Situ* Hybridization

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Sediment-hosted microbial communities pose several challenges for direct observation and precise localization of individual organisms and their metabolic functions. High-throughput sequencing sacrifices spatial context. Static measurements complicate measures of activity, and background fluorescence can obscure stains and dyes. The team addresses these challenges by developing a novel technique for microscopic mapping of metabolic networks within salt marsh sediments. Salt marshes display high levels of microbial diversity due to elevated organic matter input and active tidal cycling, supporting a wide array of metabolisms that are centered around key genes known as "functional genes." The project uses functional genes as a proxy for broader pathways that dictate biogeochemical cycling and focuses on carbon and sulfur metabolisms at the "hot spots" of plant root surfaces.

The team deploys fluorescence in situ hybridization (FISH)—a powerful tool that allows direct visual confirmation of a particular target nucleotide sequence at microscale resolution. FISH microscopy has focused on the 16S rRNA gene, providing reliable information on phylogenetic diversity but lacking information on metabolic function. Functional genes are ideal targets to elucidate pathway dynamics and putative interactions. By combining 16S rRNA gene FISH and functional gene FISH with multiplexed probe designs, researchers quantitatively link microbial diversity with putative pathway distributions in salt marsh sediments. This novel approach uses hybridization chain reaction FISH (HCR-FISH), a fluorescent technique that enhances the contrast between labeled microorganisms and the sediment matrix. Furthermore, several genes can be targeted in the same organisms, resulting in a diagnostic color code that allows the team to identify microorganisms and quantify distinct functional guilds at different distances with respect to plant roots and certain minerals. From these observations, researchers evaluate the spatial distribution of plant carbon exudate consumption, sulfur oxidation, sulfate reduction, and methanogenesis; such data allow initiation of a biogeochemical model of salt marsh sediments. More broadly, the team suggests that using multiplexed FISH with functional genes to complement 16S rRNA gene markers

is a compelling approach for mapping hot spots in complex microbial communities.

#### Investigating Redox Dynamics in Coastal Wetlands: Integrating Biogeochemical and Electrochemical Approaches at Old Woman Creek

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Redox processes in wetland environments, particularly in coastal systems like Old Woman Creek, OH, often deviate from predictions based on the traditional thermodynamic redox tower paradigm. This discrepancy is especially notable under transient hydrodynamic conditions. While redox potential (Eh) measurements provide insights, it inadequately captures the dynamic nature of microbial communities, which are central to these processes through a diverse array of catabolic reactions. To address this gap, researchers have integrated traditional biogeochemical indicators with innovative electrochemical methods, specifically zero resistance ammetry (ZRA). This study aims to (1) correlate dynamic hydrology in a freshwater terrestrial-aquatic interface wetland with redox regimes; (2) explore how redox heterogeneity influences elemental cycling at various scales; and (3) assess the effectiveness of microbial functional type representations in process-based models for capturing terminal electron acceptor stress. Researchers deployed ZRA sensors in the wetland sediment at Old Woman Creek during the summers of 2022 and 2023, alongside measurements of subsurface biogeochemical species concentrations, stratified redox sensors, and surface flux assessments. A batch reactor experiment was also conducted in 2023 for controlled observation of these processes. Preliminary findings from ZRA readings indicate significant variations correlating with water level changes and redox chemistry. These observations suggest a complex interplay between hydrology and redox dynamics, mediated by microbial activity.

Ongoing research involves aligning these findings with the process-based model ecosys. The team's goal is to evaluate the model's ability to replicate observed dynamics, particularly in representing dynamic microbial functional types and their metabolic reactions. This includes *in silica* experimental

manipulation of water levels to simulate varying environmental conditions and demonstrating the dynamic microbial terminal electron stress expressed by the consortium of microbial communities.

#### Modeling Coastal Wetland Responses to Warming and Elevated Carbon Dioxide

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Coastal ecosystems are important biogeochemical zones but have largely been ignored in Earth Systems Models (ESMs). Plant-microbe interactions drive the redox-active biogeochemical processes that structure ecosystem resilience, especially in wetlands where plant-mediated oxygen transport into the rhizosphere can stimulate aerobic microbial processes, but it can be difficult to isolate the mechanisms needed to model ecosystem responses to warming temperatures and elevated carbon dioxide ( $eCO_2$ ). As a result, SMArtX was established in 2016 to advance model representation of coastal wetland responses to global change.

Researchers have measured continuous soil redox potential in SMArtX since 2020 and found redox is consistently lower with warming and higher with  $eCO_2$ , which researchers attribute to plant-microbe feedbacks. These effects are most pronounced close to the soil surface, where the bulk of the roots are located, and illustrate the importance of rhizosphere influences on ecosystem biogeochemistry. After initial data showed a nonlinear effect of temperature on belowground root growth, researchers recently developed a simple mechanistic model of how biomass allocation responds to nitrogen supply and demand that successfully explains the field data and also reveals a surprising interaction between warming and eutrophication, predicting that enhanced nitrogen loading to marshes may reduce adverse impacts of warming on root growth.

Using a version of PLFOTRAN updated to include redox reactions relevant to coastal ecosystems, researchers found that including plant and microbial responses to *e*CO2 and temperature also more accurately represents SMArtX porewater profiles. This indicates the importance of characterizing tightly coupled vegetation-subsurface processes for developing predictive understandings as well as ongoing measurements of plant-microbe feedbacks to global change. Researchers have also recently implemented key biogeomorphic feedbacks into Energy Exascale Earth System Model (E3SM) that simulate the elevation change and productivity responses to flooding in coastal wetlands that were previously neglected. Combined with field elevation and productivity data from SMArtX, researchers will be able to determine projected wetland stability and function in response to global change.

#### Constraining Carbon Dioxide and Methane Fluxes from Diverse Tidal Wetlands: Standardizing Measurements and Analysis Across a Network of Eddy Covariance Sites in North America and Canada

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Tidal wetlands and other blue carbon (C) systems are the strongest long-term C sinks per unit area, yet these ecosystems are not well represented in Earth System Models. A Network of North American Tidal Wetlands: Understanding Through Coordinated Research Activities (NATURA) is a project that unites seven eddy covariance flux sites and aims to improve process-based modeling of these critical ecosystems. Researchers are coupling field measurements, statistical analyses, and experimental mesocosms in a model experiment (ModEx) approach to (1) improve net ecosystem exchange (NEE) partitioning into gross primary production (GPP) and ecosystem respiration (Reco); (2) quantify the influence of nitrate and salinity on GPP and Methane  $(CH_4)$  fluxes; (3) derive thresholds and responses of C fluxes to non-periodic pulses of salinity and nitrogen (N); and (4) improve biogeochemical models. An analysis comparing NEE partitioning approaches revealed that daytime partitioning deviated significantly from nighttime, artificial neural network (ANN) and stable isotope partitioning approaches. Researchers are currently testing all partitioning approaches across three sites within the network. Researchers have coupled the MEM model with an adapted version of the PEPRMT model (called PEPRMT-Tidal) with increased performance after incorporating nitrate and salinity data to help predict GPP, Reco, and CH<sub>4</sub> exchange. The GPP and Reco modules explained on average 59% of the variation in carbon dioxide (CO<sub>2</sub>) exchange with consistently low model error (normalized RMSE <1). The CH<sub>4</sub> module also explained the majority of variance in CH<sub>4</sub> emissions (54%), with an average normalized RMSE of 1.15. In Spring 2023, researchers ran mesocosm experiments demonstrating strong decreases in NEE in response

to salinity and sulfate pulses followed by rapid resilience. On the other hand,  $CH_4$  emissions significantly decreased in response to salinity and sulfate pulses with no quick recovery. Researchers are using these mesocosm data in a ModEx approach to improve modeling of the effects of nitrogen and salinity on GPP and  $CH_4$  fluxes.

### Coastal Systems National Laboratory-Led Projects

#### **COMPASS-FME**

#### Soil Bacterial Community Structure and Core Membership Along a Terrestrial-Aquatic Interface of a Freshwater and Estuarine Coastal System

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Coastal systems are dynamic environments where the intensity and duration of water exposure on soil sediments can create unique microbial niches. Microbial function is also affected by the vegetation in these systems, which vary along the coast ranging from densely vegetated upland areas to moderate and sparse vegetation in transition and wetland zones. Much of the complexity of coastal terrestrial-aquatic interfaces (TAIs) arises from the interactions among water, plants, and soils that contribute to microbial activity and biogeochemical cycling. The objective of this study was to characterize the soil bacterial communities along the coastal TAIs of a freshwater (Western Lake Erie Basin; WLE) and estuarine (Chesapeake Bay; CB) region. Soils were collected from upland, transition, and wetland transects at three sites in each region, and 16S rRNA gene amplicon sequencing was conducted. Researchers found a statistically significant effect of not only region but also transect and site on the soil bacterial communities with significant interaction effects between these factors. Within a region, the team elaborates on bacterial indicator taxa and potential functions that are uniquely associated with specific transects, as well as those taxa that are conserved across transects and defined as the "core" microbiome. Furthermore, both bacterial richness and diversity increased along the transects from upland to wetland areas in both CB and WLE. Combining these patterns with soil chemistry data, researchers found that the bacterial community in upland CB significantly correlated with phosphate ion concentration while wetland communities correlated strongly with sulfate ion concentration in both CB and WLE. Overall, the characterization of the bacterial communities across the TAIs of CB and WLE reveals important members of the soil microbiome, providing potential targets for screening in other omics datasets such as metagenomes.

#### Integrating Models and Data Across Scales to Predict Soil-Water-Plant Interactions at the Terrestrial-Aquatic Interface

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Multi-scale modeling of soil-water-plant interactions allows researchers to migrate empirical knowledge from field and laboratory studies up to a scale appropriate for a highresolution Earth system model, as represented here by the E3SM Land Model (ELM). Observed spatial variability in terrestrial aquatic interface ecosystems is represented through explicit meshes in finer-scale models, leading to subgrid parameterization in ELM. Observed ecosystem functions are represented mechanistically in finer-scale models, leading to necessary process parameterization in ELM. For this study, the approach uses multiple linked modeling platforms. 1-D and 2-D simulations are used to identify activated and permanent control points for inclusion in ELM grid-scale simulations and relationships that require further study. Researchers demonstrate that model skill has been significantly improved through incorporation of Coastal Observations, Mechanisms, and Predictions Across Systems and Scales (COMPASS) data in fine-scale simulations, and that this has translated to improved prediction skill at larger spatial scales in ELM. Researchers show that migrating to E3SM-relevant scale requires data with improved temporal resolution, and more information on belowground dynamics.

Model connections between hydrology, biogeochemistry, and ecohydrology are explored to inform ELM-ATS-PFLOTRAN coupling as a common framework. This effort connects directly to ongoing development in COMPASS-Great Lakes Modeling (GLM) and Interoperable Design of Extreme-scale Application Software (IDEAS)-Watersheds projects.

#### Geophysical Imaging for Scaling Understanding of Hydro-Biogeochemical State Changes Across Coastal Interfaces

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Geophysical methods provide highly resolved spatial images of responses sensitive to subsurface state changes and can be used to monitor subsurface hydrology at a continuous spatiotemporal scale. However, extracting quantitative hydrological and biogeochemical information from geophysical images remains challenging. This study uses repeated measurements of natural and induced electrical potential fields to quantify changes in soil moisture, salinity, and redox potential at coastal interfaces along the Chesapeake Bay and Lake Erie. At the Chesapeake Bay, researchers used petrophysical models derived from laboratory multisalinity electrical measurements to estimate changes in soil moisture and fluid salinity from electrical resistivity and induced polarization measurements during a simulated flooding experiment. The experiment was conducted across two hydrologically isolated 2,000 m<sup>2</sup> plots simultaneously inundated with freshwater and estuarine water. Time-lapse electrical resistivity and induced polarization measurements were used to image the propagation of the infiltration front. The team used a modified Archie's law to estimate changes in soil moisture and salinity in response to the simulated flooding event. Researchers found that the geophysical methods could capture the propagation of the infiltration front through changes in bulk electrical conductivity over time. Additionally, significant changes in imaginary conductivity were observed only in the estuarine plot, which correlated with the increasing soil salinity. Estimates of the soil moisture and salinity contents from the resistivity and induced polarization datasets agreed with measurements from *in situ* soil sensors. At the Lake Erie area, researchers used repeated co-located measurements of natural electrical currents (Self-Potential) and redox potential to show that the electrochemical contribution of Self-Potential correlates with redox potential, providing an alternative approach to estimate spatial changes in soil redox potential. The results of this study extend the use of geophysical imaging for improving spatial estimates of soil moisture, salinity, and redox potential changes across coastal interfaces.

#### Exploring the Impact of Seawater Infiltration on Coastal Biogeochemistry: An Integrated Modeling Study of the Terrestrial Aquatic Interfaces

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As the climate and environment continue to change, a comprehensive and predictive understanding of coastal terrestrial aquatic interfaces (TAIs) is increasingly critical. In this study, researchers investigate the impacts of seawater infiltration on the biogeochemical dynamics of coastal TAIs in the Chesapeake Bay region. An integrated approach that combines hydrological, biogeochemical, and vegetation dynamics models is applied along a gradient from coastal wetland marsh to upland forest. The Advanced Terrestrial Simulator (ATS) is used to simulate water flow, incorporating overland and subsurface dynamics under various scenarios. Outputs from the ATS, specifically water level and salinity data, are then fed into the FATES-Hydro model to predict vegetation responses to shifting hydrological conditions. These predictions include key parameters such as leaf fall and leaf area index, which are then used to refine the ATS simulations.

Additionally, the PFLOTRAN model, coupled with ATS through Alquimia, simulates biogeochemical processes considering the altered water table, microbial activity, salinity, and plant community dynamics due to seawater infiltration. These results show that dynamic seawater levels have a strong influence on dissolved oxygen and salinity in coastal TAIs. Dynamic changes in the oxygenated zone directly affected soil redox conditions and biogeochemical processes. Notably, higher salinity was associated with lower aerobic reaction rates and higher dissolved organic carbon content, suggesting that salinity plays a key role in regulating microbial activities and chemical reactions. In addition, the introduction of dissolved organic carbon (DOC) from degrading vegetation significantly altered local redox processes, suggesting a complex interaction between biogeochemical processes and vegetation dynamics. These results highlight the critical importance of integrated modeling in understanding the multiple impacts of seawater infiltration on coastal TAIs. Through this integrated approach, researchers gained a detailed understanding of the complex

interactions occurring across coastal TAIs, enhancing the knowledge of their response to environmental change.

#### A Tale of Two Scales: Soils Across Coastal Terrestrial-Aquatic Interfaces

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Regional variability, local hydrological gradients, and complex interconnections make soils at the coastal terrestrial-aquatic interface (TAI) extremely difficult to characterize, simulate, and thus predict responses to future hydrological regimes. The team characterized soil biogeochemical parameters across the TAI in contrasting freshwater (western Lake Erie Basin) and estuarine (Chesapeake Bay) coastal systems. Researchers established transects at three sites in each region to capture: (1) upland forests, the terrestrial endmember; (2) transition forests with intermittent inundation; and (3) wetlands, with persistent inundation. Along each transect, soils were analyzed for physical and chemical parameters, including elemental composition, extractable nutrients and ions, water retention and particle size. At regional scales, freshwater and estuarine soils varied strongly in their biogeochemical controls and variance structures. The Lake Erie soils had elevated phosphate and nitrate concentrations and showed evidence of redox-driven sulfur cycling. The Chesapeake Bay soils, on the other hand, showed the impact of seawater encroaching into the uplands, with evidence of significant iron redox dynamics across the transects. At transect scales, uplands, transitions and wetlands differed in their soil biogeochemical drivers. Surprisingly, transitions were not the mid-point or average of adjacent uplands and wetlands. Transition soils in Lake Erie showed higher SOM and phosphate concentrations than upland and wetland, suggesting that the transition may be a hotspot for certain nutrients. Furthermore, researchers hypothesized that transition soils would have higher variance in soil biogeochemical variables but this was not supported across regions. While transition soils did have the highest variance in Western Lake Erie, wetlands had the highest variance in the Chesapeake Bay, likely due to tidal

influences. This multi-scale characterization of TAI soils is a necessary first step for scaling and predictions, particularly as punctuated (storms, seiches) and gradual (lake level change and relative sea level rise) disturbances alter hydrological conditions across the TAI gradient.

#### Biogeochemical Controls Vary Across the Upland to Wetland Gradient of Two U.S. Coastal Regions: Results from the EXCHANGE Consortium

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The Exploration of Coastal Hydrobiogeochemistry Across a Network of Gradients and Experiments (EXCHANGE) Consortium, a component of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales-Field, Measurements, and Experiments (COMPASS-FME) project, synthesizes knowledge related to hydrologically and biogeochemically dynamic coastal terrestrial-aquatic interfaces (TAIs), with the aim to quantify coastal ecosystem heterogeneity across transect and regional scales. The consortium, comprising diverse researchers based around the U.S. Great Lakes and Mid-Atlantic regions, fosters interdisciplinary and synergistic collaborations. During the commencing campaign, EXCHANGE Campaign 1 (EC1), open-access datasets were generated, encompassing geochemical, physicochemical, and organic matter characterizations with interoperable metadata. These resources empower the community to pose new questions and gain insights by contextualizing information across diverse sites and regions. Notably, EC1 data revealed significant spatial variability in soil carbon content, with region, transect location, and soil pH serving as key predictors of soil carbon. Contrary to the hypothesis, transition zones did not exhibit the anticipated highest variability in soil carbon content. The drivers of greenhouse gas production from soils and sediments incubated in seawater were contingent on the originating transect location from across the TAI, suggesting potential biogeochemical feedbacks as inundation regimes shift inland.

In the ongoing EXCHANGE Campaign 2 (EC2), researchers explore how prolonged flooding affects the turnover of soil microbial carbon pools, specifically examining whether carbon starvation or terminal electron availability drives these events. Additionally, to assess how local drivers influence upland-to-wetland conversion, researchers investigate the relationship between soil and water characteristics, elevation, and rates of land conversion inferred from remote sensing data. The outcomes of the EXCHANGE project are integral to validating input parameters for biogeochemical models, contributing to a predictive understanding of coastal biogeochemical function.

#### A Processing Pipeline for High-Volume, High-Quality Environmental Sensor Data

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The Coastal Observations, Mechanisms, and Predictions Across Systems and Scales-Field, Measurements, and Experiments (COMPASS-FME) project has a network of observational sites across the Chesapeake Bay and western Lake Erie regions, extensively instrumented with soil, vegetation, and weather sensors logging data every 15 minutes. Such high-resolution environmental monitoring requires sophisticated data management in order to provide quality, timely data to researchers and the public. COMPASS-FME is organized around Findable, Accessible, Interoperable, and Reusable (FAIR) data principles and prioritizes rapid model-experiment iteration, and thus a major goal is to make this site sensor data rapidly available for quality assurance/quality control (QA/QC), analysis, and model ingestion, and openly available on ESS-DIVE within 1 year of collection. A combination of hardware and software workflows makes this possible. Sensor data are automatically uploaded to Smithsonian Environmental Research Center and Dropbox servers. A multi-step processing pipeline assigns a unique hash to each observation, ensuring traceability; reformats and unit-transforms the data; flags out-of-bounds of outof-service problems; propagates quality flags based on the physical site setup; and automatically generates extensive site-specific metadata. The pipeline runs in R and uses technologies such as Quarto for logs and documentation; a SQL database for data quality flags; automated code testing; and both algorithmic and human QA/QC. Data are released in L0 (close to raw), L1 (limited QA/QC, full metadata),

and L2 (highest quality, filtered and averaged) levels. This open-source system runs on the COMPASS computing cluster and processed over half a billion raw observations to produce the recent v1.0 data release of 97.3 million observations over 2 years.

#### Responses to Flooding in a Coastal Forest: Insights from the TEMPEST Landscape-Scale Manipulation Experiment

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Flooding of coastal forests is predicted to increase with rising seas and higher frequency and intensity of extreme weather. Because flooding increases soil saturation and sometimes salinity, extreme precipitation or storm surge may impact forest health and soil biogeochemistry. However, it is difficult to quantify relationships between soil saturation, salinity exposure, and ecosystem function because flooding driven by sea-level rise is occurring across decadal scales and flooding driven by storms is difficult to predict and therefore difficult to measure. To address these challenges, the team subjected 50m x 40m experimental plots in a coastal forest in Maryland, U.S., to fresh and estuarine water inundation events equal to precipitation from a ~10 year return interval storm for a duration of 10 hours as part of the Terrestrial Ecosystem Manipulation to Probe the Effects of Storm Treatments (TEMPEST) experiment over multiple years. Researchers present a synthesis of ecosystem responses to flooding during the first flooding event, TEMPEST 1 (2022), where researchers found immediate and clear responses to flooding and salinity from the geosphere to the atmosphere with variable return times for biogeochemical, hydrologic, and vegetation variables. During TEMPEST 2 (2023), based on findings from TEMPEST 1, researchers installed in situ dissolved oxygen and redox sensors in the upper soil profile and applied two sequential flood treatments. Researchers found that saturation drives short-lived anoxia throughout the top 30 cm of the soil column in both treatment plots, which recovered to antecedent oxygen conditions within hours post-event near the surface but days at depth. Decreased redox potential persisted for

more than a week following inundation, indicating that flooding has prolonged effects on ecological and soil biogeochemical processes. Together, these results provide quantitative, spatiotemporally resolved insights into the impacts that increasing inundation regimes will have on coastal forest health and function.

#### Coastal Flooding Redistributes Water Dispersible Colloids Impacting Dissolved Oxygen Dynamics

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Coastal soils are increasingly impacted by hydrologic intensification in the form of rising ocean waters and floods from storm surges and precipitation. Alternating salt and freshwater has the potential to disperse mineral and organic colloids, which can lead to disintegration of soil structure and clogging of pore spaces and can reduce important functions like infiltration and gas exchange. Additionally, colloids are important to carbon and nutrient cycling, potentially influencing biological oxygen demand. To investigate the oxygen dynamics in repeatedly flooded soils, the team conducted a series of laboratory-based flood simulations on intact soil cores from an A and B horizon collected from the toe slope of an upland forest at the Smithsonian Environmental Research Center, Maryland, U.S. The team subjected the cores to 24 hours of saturation with saltwater from the Rhode River estuary followed by 24 hours of saturation with freshwater, with a 24-hour draining event in between flood events. Significant changes were found in pore size distribution, significant redistribution of colloids, and the A horizon became sodic after three saltwater floods. During draining, oxygen diffusion into soil was reduced for saltwater flooded soils, likely due to clogging of smaller pores. The team also found that oxygen consumed varied between soil horizons relative to water dispersible suspension fraction and that of the bulk soil. Researchers concluded that a relatively small number of saltwater flooding events can induce a measurable change in soil physical properties, impacting the biogeochemical dynamics of the soils.

#### Coastal Terrestrial-Aquatic Interfaces: Iron Biogeochemistry in the Great Lakes and Chesapeake Bay Regions

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Coastal terrestrial-aquatic interfaces are dynamic environments with hydrological fluctuations that drive the coupled biogeochemical cycling of carbon, nutrients, and redox sensitive elements such as iron (Fe). As part of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales-Field, Measurements, and Experiments project, the aim is to better understand Fe biogeochemistry in coastal ecosystems, in order to better predict global biogeochemical changes in response to hydrological disturbances. Researchers combined X-ray Absorption Spectroscopy with mineralogical, solid phase, and pore water chemistry analyses to study Fe cycling across upland to shoreline gradients along the Lake Erie (freshwater) and Chesapeake Bay (estuarine) coasts. Researchers show that Fe occurs mainly in its oxidized form, Fe(III), in cores collected from unsaturated upland and transition locations, with variable proportions of Fe(III)-oxyhydroxide, Fe(II,III)-phyllosilicate, and Fe(III)-organic species depending on the soil characteristics (e.g., mineral and organic carbon contents). In water-saturated soils (i.e., wetlands and some transition zones), Fe(III)/Fe(II) ratios and Fe(II) species in the solids indicated diverse redox and biogeochemical conditions. At the Lake Erie wetlands, Fe reduction was identified as a dominant biogeochemical process, controlling the release of Fe(II) in the pore waters.

Nevertheless, the extent of Fe(III) reduction was limited by the presence of recalcitrant Fe(III) in phyllosilicates. In the Chesapeake Bay wetlands and one transition site, pore water sulfide concentrations and the abundance of pyrite (FeS<sub>2</sub>) indicate that Fe cycling is controlled by sulfur- driven redox dynamics. In contrast, other transition sites at both Lake Erie and Chesapeake Bay showed predominantly oxidized Fe(III) despite water-saturated conditions. At these sites, the pore water chemistry was indicative of little to no reduction of Fe(III) and sulfate, suggesting that water inputs may have impacted microbial redox processes.

#### Biogeochemistry and Function Across the Terrestrial-Aquatic Interface: Transition Zones Present Unique and Non-Conservative Behavior

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#### https://compass.pnnl.gov/FME/COMPASSFME

Coastal ecosystems are dynamic transition zones between land and water, spanning shoreline, wetland, and upland ecosystems that compress and expand in response to tides, lake-level changes, weather, and climate. Changes to inundation regimes significantly alter carbon cycling and soil biogeochemistry of coastal terrestrial aquatic interfaces (TAIs).

Understanding these shifts and the major drivers of ecosystem function is critical to representing and predicting change in coastal TAI biogeochemistry. As a part of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales-Field, Measurements, and Experiments (COMPASS-FME) project, researchers installed in situ sensor networks and conducted high-resolution monitoring of the interactions among water, soil, and plants to determine how biogeochemical cycling of carbon and nutrients shift across the TAIs in response to shifting inundation regimes. Seven field sites were established with transects spanning upland forests, stressed forests transitioning to wetland, and herbaceous wetland to capture temporally dynamic behaviors across diverse coastal systems in the Chesapeake Bay and Great Lakes regions. At each site, monthly measurements of soil methane fluxes, redox profiles, conductivity, and porewater constituents were made. In the Chesapeake Bay, soil redox potential decreased along gradients from upland forest to wetland, and soil conductivity and porewater sulfate concentrations increased. In both regions, wetland zones had the highest methane  $(CH_4)$  emissions, with diminished CH<sub>4</sub> uptake in transitional forests prior to tree mortality suggesting that: (1) soils respond more rapidly than vegetation to changing hydrological regimes; and

(2) flooding exerts stronger control on CH<sub>4</sub> than terminal electron acceptor abundance (e.g.,  $SO_4^{2-}$ ). These results suggest that transition zone soils don't simply fall between wetland and upland endmembers; they have unique properties. This has important implications for understanding the impacts of changing inundation on greenhouse gas emissions and carbon storage along the terrestrial-aquatic interface at the ecosystem scale.

#### AquaMEND: Reconciling Multiple Impacts of Salinization on Soil Carbon Biogeochemistry

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#### https://compass.pnnl.gov/FME/COMPASSFME

Soil salinization exacerbated by climate change poses a global threat to ecosystem function and soil quality. Despite extensive research, consensus on the impact of salinity on belowground carbon cycling remains elusive, hindering accurate predictions. Salinity influences carbon cycling through direct effects on microbial activity and indirect alterations to soil physicochemical properties. Current models inadequately represent the interplay of salinity, cation exchange, pH, and soil organic carbon availability, relying on linear reduction functions that overlook specific physicochemical changes induced by salinity. To address this gap, researchers propose an integrated model framework, AquaMEND that combines microbial-explicit and aqueousexplicit geochemical models. This model's explicit salinity module captures salinity-induced cation exchange and surface complexation, important processes governing solute chemistry and nutrient availability in soils, which offers a substantial leap towards more realistic and dynamic simulations of soil salinity change and solute behaviors. Coupling with salinity response functions, researchers have derived to capture the salinity impact on both salt-sensitive and saltresistant microbial processes and are able to simulate how the abiotic and biotic mechanisms work individually and collectively to regulate various organic and inorganic pools and fluxes.

The parallel structure of aqueous and non-aqueous phases, together with an energetic framework to consistently build microbial functions and associated physiological traits, making this model highly flexible and versatile in solving dynamic coupling of organics, minerals, and microbes under various environmental settings.

#### **Integrated Coastal Modeling**

#### Integrated Coastal Modeling: ESS Modeling of Natural Watersheds and Engineered Systems in the Coastal Zone

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#### https://icom.pnnl.gov

The Integrated Coastal Modeling project brings together four programs within BER, namely Regional and Global Model Analysis, Earth System Model Development, Multi-Sector Dynamics, and ESS. This unique collaboration offers the opportunity to explore various facets of coastal science in an interdisciplinary setting. The project's ESS contributions consider coastal regions as comprised of a range of natural and engineered features that play a critical role in determining their resilience to various climate-influenced drivers, including drought, sea level rise, storm surge, and shifting precipitation patterns. In this setting, the full coupling of surface and subsurface processes is critical to developing a predictive understanding of how these systems function. To demonstrate this benefit of fully coupled process-based models, the team used the Advanced Terrestrial Simulator (ATS) to study the impact of antecedent conditions on flooding through the response of the Harbeson watershed to a series of storms. Next, to continue exploring the natural system response, researchers used the saltwater intrusion capabilities in the ATS to study the formation of ghost forests in the Delaware Bay. This capability also supports studies related to salt marsh migration and the loss of agricultural land to saltwater intrusion. Finally, to study the engineered environment and its response to these drivers, the team highlights a prototype of a storm drain network process kernel in the ATS that is coupled to its integrated hydrology model. This fully coupled system has the unique capability to not only capture the impact of the drainage network on flooding, but also the impact of green spaces or riparian zones. The project demonstrates this new urban modeling capability in a synthetic setting. In future work, the team will consider specific sites with data supporting green space performance assessments under flooding and storm drain networks inferred from publicly available data.

### Urban-Influenced Coastal Systems DOE Early Career Projects

#### Urban Resilience Across the Terrestrial-Aquatic Continuum

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The impacts of urbanization on ecosystem functions remain ambiguous, leading to uncertainty in urban carbon cycling within Earth systems models. To address this knowledge gap, the project investigates the overarching hypothesis that commonalities in microbial functions lead to distinct conserved biogeochemical processes in the urban environment. The team will present data-driven investigations of urban coastal resistance to precipitation across the United States and global urban soil microbiomes, as well as preliminary results from surveys of organic matter cycling in the Baltimore and Duluth-Superior metropolitan areas. By calculating a resistance index based on dissolved oxygen, the project uncovers factors influencing coastal resistance to extreme precipitation at the continental scale and reveals that estuaries with higher urban influences seem to be more resistant to precipitation events—a result that is counter to the team's initial hypothesis. At smaller scales, the factors influencing resistance interact with estuarine salinity and vary across individual estuaries, where researchers find relationships of resistance with additional factors. Considering escalating stressors along urban coastlines, these results are important for informing decisions regarding process-based model representations and estuarine water quality.

The project also uses existing urban soil microbiomes to assess changes in microbial phylogeny and functional potential across the urban environment and to derive a core urban microbiome for process-based model development. The team finds that functional potential is largely correlated to microbial phylogeny at the order-level, regardless of geographic location. Ubiquitous energy-generating pathways leverage the Calvin cycle as well as metabolisms based on nitrogen oxidation and reduction. Core organisms include many members of *Pseudomonadota* with diverse metabolisms, as well as archaea known to be involved in methane and nitrogen cycling.

Collectively, this project will create a unique knowledge set inclusive of control points, microbial decomposition processes, and their relationships to various urban attributes that influence the response of coastal zones to environmental extremes.

### Redox Response to Hydrologic Variability in an Aggrading Coastal Delta

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http://herndongeochemistry.com

Coastal ecosystems serve as the interface between land and oceans, processing material that is delivered by rivers and buffering interior lands against sea level rise and hurricanes. The biogeochemical function of these ecosystems is not well represented in Earth system models, limiting prediction of how ecosystem processes vary over time and respond to chronic and episodic disturbance. The project's objective is to understand how soil biogeochemistry varies across redox gradients shaped by landscape features and variable hydrology. Here, researchers evaluate how redox processes respond to changing water levels on the freshwater Wax Lake Delta, one of the few aggrading areas of coastal Louisiana. The team examines these processes across two elevation transects spanning supra- to subtidal zones that are located on older and younger portions of a deltaic island. Sensor networks continuously record water level, soil redox potential, soil moisture, pH, and conductivity. Soil and pore water are collected seasonally to evaluate carbon and (micro)nutrient storage and mobilization. Researchers determine that soil redox  $(E_b)$  responds to water tables that fluctuate with the seasons and tides. On the old transect, surface soils (<20 cm) in supra- and intertidal zones transitioned from reducing (<0 millivolts at pH 7) to oxidizing conditions during summer as water tables dropped >0.5 m below the soil surface. On the young transect, E<sub>h</sub> in supraand intertidal surface soils fluctuated with tides. Subtidal soils and deeper soils were persistently reducing. Soil water contained high dissolved iron (Fe<sup>2+</sup>), manganese (Mn), and ammonium but low sulfate and nitrate, indicating microbial reduction of Fe and Mn oxides, sulfate, and nitrate.

Dissolved phosphate also increased with depth and was correlated with dissolved Fe, indicating phosphate release from dissolving Fe oxides. This work provides insight into the spatial and temporal variability of biogeochemical processes in a freshwater wetland.

#### Student

#### Assessing Greenhouse Gas Structural and Functional Resilience of Freshwater Coastal Wetlands Subject to Persistent Saltwater Intrusion Events

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Acute saltwater intrusion (SWI) events, often triggered by storm surges during high-intensity hurricanes, significantly impact the dynamics of freshwater wetlands. This study focuses on patches dominated by Typha domingensis and Panicum hemitomon, two prevalent wetland species in freshwater wetlands of the northern Gulf of Mexico, and investigates their physiological and functional response to acute SWI events in different durations of 1-, 3-, and 5- days with an approximate 2 practical salinity unit (PSU) concentration in an experimental wetland ecosystem complex following a before-after impact control experimental design. Measurements of methane  $(CH_4)$  fluxes, carbon dioxide  $(CO_2)$  fluxes, and soil porewater concentrations (5-, 10-, 20-cm depths), and spectral indices [normalized difference vegetation index (NDVI), photochemical reflectance index (PRI), plant senescence reflectance index (PSRI)] had diverging responses from two ecohydrological patches. In the T. domingensis patches, fluxes were not affected by the three SWI events. Porewater concentrations remain unaffected as well, regardless of the SWI duration except for CH<sub>4</sub> concentrations at 20 cm soil depth, which increased after the 5-day SWI.

NDVIs decreased only in the 3-day SWI, but PRI and PSRI were similar before and after the SWI events. In the P. hemitomon patch, CO<sub>2</sub> fluxes (*i.e.*, emissions) decreased after the 3-day treatment, whereas CH<sub>4</sub> fluxes did not change. The team also observed a decrease in the CO<sub>2</sub> porewater concentration at the 20-cm depth, but no changes for CH<sub>4</sub> concentrations. Again, the PSRI and PRI remained unchanged after SWI events, but surprisingly, the NDVI increased during the 1-day SWI event. These results support the resiliency of T. domingensis and susceptibility of P. hemitomon. Increasing the salinity may challenge the resiliency to low disturbances and give insight on further adaptational physiological and functional responses. The next steps in this research include analyzing data from a similar threelevel duration experimentation for five PSU-simulated SWI events: a new field campaign to evaluate variable responses to longer inundation periods.

# Urban

Urban research is advancing the science underpinning the understanding and predictability of urban systems and their two-way interactions with the climate system. This knowledge will help inform equitable climate and energy solutions that can strengthen community-scale resilience across urban landscapes.

## Urban National Laboratory Project

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

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https://www.ornl.gov/project/ biogeochemical-processes-influencing-urban-ecosystems

Urban microclimate varies spatially with degree of urbanization and vegetation composition. Residents in wealthier neighborhoods often have more green space and tree canopy cover than low-income communities (e.g., <\$50,000 annual household income), leading to less extreme summer temperatures. The urban heat island effect thus impacts low socioeconomic households with increased heat stress and air conditioning costs. Consequently, heterogeneities in tree canopy cover and urban heat island effects can result in environmental injustice due to unequal distribution according to income and race. The goal of this project is to understand how temperature and relative humidity in an urban area are affected by plant evapotranspiration and soil moisture dynamics. The project hypothesizes 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 cooling in the winter. The team selected Knoxville, TN, for a coupled model-experiment pilot investigation based on a representativeness analysis of cities in the eastern United States. Researchers used geospatial information coupled with socioeconomic data such as population density, race, and income to select six urban parks that vary in temperature, tree canopy cover, imperviousness, and topography. Each site was instrumented to measure soil water, soil and air temperature, relative humidity, and solar radiation. Sap flow sensors were installed into representative trees at each site. The data will be used to determine relationships between urban microclimate and natural and built urban components as a function of diurnal and seasonal conditions. The team also uses pertinent observations to assess the capability of the E3SM Land Model to delineate the interplay between urban microclimates and natural ecosystems, such as soils and plants, across varying levels of urbanization.

# Climate Resilience Center

Climate Resilience Centers will improve the availability and utility of BER research, data, models, and capabilities to address climate resiliency, particularly by underrepresented or vulnerable communities.

### Southwestern Mountains Climate Resilience Center

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https://nau.edu/forestry/smcrc/

The Southwestern Mountains Climate Resilience Center (SMCRC) was established to address fundamental and applied research needs of regional populations in highlands of the southwestern United States. The communities and stakeholders of the southwestern highlands include the highest density of Native American populations and Tribal lands in the United States. Key local challenges in this region include drought, fire, flooding, and insect herbivory that lead to ecosystem degradation and high socioeconomic burdens on rural and Tribal communities. These factors are exacerbated by warming climate, requiring a forward-looking approach to reducing damage through climate-adaptive management. The SMCRC's objectives are to (1) integrate research tools in dynamics of forests, disturbances, climate, carbon, and hydrology that provide informative practical examples for climate-resilient management of public and Tribal lands; (2) develop an outreach program for science translation reaching K-12 and adult populations through online materials and a network of Native-serving teachers; (3) foster training and science translation of multidisciplinary climate scientists by building on links with a community college, Tribal college, the national-scale Institute for Tribal Environmental Professionals, and the Southwest Fire Science Consortium; and (4) partner with DOE scientists on developing and communicating relevant science in two-way interactions with southwestern communities. To date, the SMCRC team has established relationships with partners, finalized the job search for a research coordinator, and initiated approval of instrumentation for a local field site at the Fort Valley Experimental Forest near Flagstaff, AZ.

# Crosscutting Resources

BER scientific user facilities, community research infrastructure, community databases, and analytical tools enable mission-relevant Earth system science, advance scientific discovery, and broaden the impact of Environmental System Science-supported research.

### Molecular and Microstructural Soil Characterization User Program and Soil Data Across the Contiguous United States: EMSL's Molecular Observation Network

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Standardized soil molecular and microscale data is urgently needed at regional and larger scales to improve biogeochemical process representations, provide model inputs, and reduce uncertainty in Earth system and climate predictions. The Environmental Molecular Sciences Laboratory's (EMSL's) Molecular Observation Network (MONet) is addressing this gap through a distributed open science program that provides numerous benefits to researchers, including:

- Researchers submitting soil cores for analysis receive
   ≥ 30 data advanced types, including soil organic matter
   high-resolution composition, 3D pore structure char acterization, metagenomes, and a suite of conventional
   biogeochemical parameters, at no additional cost to user
   scientists
- Access to molecular and microscale soil data across the continental U.S. in the MONet database
- Extensive training opportunities about the fundamentals of MONet data types and how to use them in graduate, postdoctoral, and career scientist research
- Networking and interacting with a growing community of MONet open science colleagues

Scientists participating in MONet Soil Function user research calls gain access to EMSL's premier high-resolution molecular and microstructural characterization capabilities including, Fourier Transform Ion Cyclotron Resonance (FT-ICR) mass spectrometer and X-ray computed tomography, and Joint Genome Institute's metagenome sequencing and annotation workflows. MONet soil analyses follow standardized workflows that enable high consistency and throughput that reduce uncertainty in data. The resulting data are open to the scientific community in a searchable findability, accessibility, interoperability, and reusability (FAIR) database, explorable using online data visualization and processing tools, and supported by training and community engagement programs. MONet is developing tools and scaling functions to enhance data accessibility and utilization for a range of biogeochemical process and Earth system models.

### Opportunities for Rhizosphere Function, Biogeochemistry and Terrestrial-Atmospheric User Research at the Environmental Molecular Sciences Laboratory

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### https://www.emsl.pnnl.gov

The Environmental Transformations and Interactions Science Area at the Environmental Molecular Sciences Laboratory (EMSL) provides best-in-class instrumentation and expertise for external users to investigate cycling, transformation, and transport of critical nutrients, elements, and particles at molecular and microstructural scales. Improved knowledge of these areas is critical to improving Earth systems and climate models. Researchers are focused on systems-scale research in the following three areas:

**Rhizosphere Function** investigates the impact of root system architecture and rhizodeposition on the molecular and structural mechanisms root-soil-microbe interactions. The goal is to improve prediction of root-controlled processes and their impacts on plant resilience, nutrient cycling, and volatile emissions under environmental changes. Key capabilities include phytotrons, caron (C) flux measurement using isotope ratio mass spectrometry (IRMS) and nanoscale secondary ion mass spectrometry (NanoSIMS), micromodels, multiomics, metabolite imaging, and nondestructive root system imaging.

**Terrestrial-Atmosphere Processes** investigates emission mechanisms of aerosols and gases from plants and soil into the atmosphere and the subsequent formation of particles, with a focus on multiphase aerosol interfacial chemistry and aging processes near Earth's surface and extending up to the atmospheric boundary layer. Research also focuses on how aerosols participate in warm and cold cloud formation by acting as cloud condensation nuclei or ice nucleating particles and how these impact Earth's radiative budget and aerosol deposition on terrestrial ecosystems.

**Biogeochemical Transformations** investigates the interplay of geology, chemistry, and biology to understand molecular/microscale mechanisms of biogeochemical transformations of C, nutrients, and minerals. User research directly supports improvement of biogeochemical process representations, process scaling from molecularto-landscape, and predictive Earth system models. Key capabilities include X-ray computed tomography, helium ion and scanning electron microscopy, mass spectrometry compound identification and imaging, and Mössbauer, X-ray photoelectron, and nuclear magnetic resonance spectroscopy.

EMSL is a DOE Office of Science user facility.

### ESS-DIVE: Enabling Integration Across Diverse Environmental Systems Science Data

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https://ess-dive.lbl.gov

The ESS Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) is a data repository designed for the U.S. DOE's ESS program. ESS-DIVE enables collection, storage, management, and sharing of a variety of observational, experimental, and modeling data generated across the program. The volume, complexity, and diversity of these interdisciplinary data present unique integration challenges.

Researchers discuss how ESS-DIVE approaches data integration across these datasets and with other data systems.

Metadata in ESS-DIVE are published in a number of formats, including the JSON-LD format, which allows the data to be easily ingested and understood by external systems (e.g., Google Dataset Search, OSTI, Data.gov etc.). ESS-DIVE provides a systematic method for linking datasets from other recognized data providers. This allows metadata to be searchable in ESS-DIVE, while linking out to externally managed data products. In order to track and relate sample data across systems, researchers encourage the use of common standards for sample data identifiers, such as the International Generic Sample Number (IGSN). ESS-DIVE works closely with ESS Scientists to promote adoption of standard data reporting formats, which researchers are using to develop tools for data validation, advanced search within data files, and data synthesis.

ESS-DIVE offers project-specific features that allow researchers to collaborate and share data within their teams efficiently. Project data portals allow you to create a collection of project datasets along with contextual information, making project data more findable and accessible. ESS-DIVE also supports a secondary storage layer to serve very large, hierarchical datasets. This allows users to directly browse and access large volumes of data over the web, and efficiently move data between sites using a highperformance data transfer service–Globus. ESS-DIVE is integrated with DataONE, a federation of interoperable data repositories facilitating open science and data discovery.

### Improvements to Knowledgebase Platform Toward Causal Predictive Ecology

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### https://www.kbase.us

Given the focus of DOE BER programs on environmental ecology, Knowledge Base (KBase) has prioritized predictive causal ecology as its scientific target. Working with DOEfunded collaborators, researchers integrated a set of tools within KBase that capture many of the steps required to support a mechanistic understanding of environmental system behavior (Figure 1). Over the past year, in partnership with many projects, the team made significant progress implementing and improving many steps in the causal ecology workflow. This begins with improving the mechanisms for predicting the protein content of an environment based on metagenome-assembled genomes (MAGs) and amplicon sequence variant (ASVs). Researchers now have tools to map these entities to reference data to produce probabilistic predictions of what functions are present and how they are distributed among species in the environment. The team will show how this work has been applied to datasets from Genome Resolved Open Wetlands (GROW) and the Joint Genome Institute (JGI) to improve MAG quality and produce improved strain models. Once researchers have improved understanding of the protein content of a strain within an environment, the team next wants to produce a metabolic model of each strain to predict its behavior. Using an upgraded ModelSEED2 pipeline for model

reconstruction, researchers significantly improved capacity for predicting energy biosynthesis strategies; improved templates for representing cyanobacteria, archaea, and bacteria; tailored biomass formulations based on metabolic network analysis; and improved predictions of organism metabolic properties like auxotrophy. Researchers are also developing enhanced tools for predicting strain phenotypes and exploring the synergy between machine-learning predictions and metabolic modeling. Finally, by combining strain models into community metabolic models and integrating multiomics data, the team can predict and contrast the active pathways and species interactions to discover patterns of variation with environmental parameters. The team will demonstrate these capabilities with narrative notebooks illustrating each workflow that is currently available.

### The National Microbiome Data Collaborative: A Community-Driven Data Infrastructure

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### https://microbiomedata.org

Microbes play a key role in many environmental processes. Microbiome data is multifaceted, encompassing molecular/ omics data (sequence, metabolic, proteomic, natural organic matter) as well as biogeochemical. Organizing and integrating this data presents many technological and organizational challenges. The DOE National Microbiome Data Collaborative (NMDC) was created to tackle interdisciplinary environmental microbiome science by connecting data, people, and ideas.

The NMDC provides three core products for microbiome scientists: A user-friendly web interface for submitting data and metadata about collected samples, a platform for analyzing sample omics data, and a web portal that allows members of the community to explore and collate datasets, using either a web interface or Application Programming Interfaces (APIs).

NMDC is committed to the "FAIR" principles to make data Findable, Accessible, Interoperable, and Reusable. Each piece of information in the NMDC database, from the source sample through to processed data objects, is assigned a unique, persistent, resolvable identifier. Sample metadata follows the Genomic Standards Consortium standards, and terms from the Environment Ontology (ENVO) are used to annotate sample environments. The unified data model weaves together these standards, organized around core concepts (e.g., studies, samples, analytes, computational workflows, data objects, gene functions), as well as different properties (e.g., soil moisture content, pH, metabolite concentration, etc.). Researchers are developing a Field Notes mobile application that allows for real-time sample collection.

The NMDC has a number of partnerships with other organizations. An example is the partnership with the NSF National Ecological Observatory Network (NEON) to provid e access to paired metagenome and environmental data. Using NMDC APIs it is possible to explore relationships between metagenome features such as taxonomic community and NEON environmental variables, or to combine with other datasets to perform larger meta-analyses.

Together, the NMDC is advancing how scientists create, use, and reuse microbiome data.

## Research Development and Partnership Pilots

BER Earth and Environmental Systems Sciences Division's (EESSD) RDPP projects are part of an effort to broaden and diversify institutional representation in the EESSD portfolio with institutions that have limited familiarity or engagement with EESSD-supported efforts.

### Virtual

### Advancement of High-Resolution Microfluidic Device in Atmospheric Ice Nucleation Research and Integration into Science Teaching

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Ambient ice-nucleating particles (INPs) constitute a crucial subset of aerosol particles, playing a vital role in the heterogeneous formation of ice crystals under ice supersaturation conditions. However, uncertainties persist in understanding aerosol radiative forcing and feedback associated with INPs. The research addresses the challenge of comprehending atmospheric ice formation in mixed-phase clouds where immersion freezing is the dominant mechanism. This motivates the community's interest in quantifying and improving prognostic skills for INP number concentrations. To address these gaps, an affordable, offline microfluidic freezing assay system was developed to measure INP concentration. The system's performance was verified using known ice nucleation active compounds in immersion mode and high-latitude soil samples. Two novel microfluidic droplet trapping circuits featuring static droplet arrays with 60 interconnected loops (15 nanoliters) and 720 loops (1.5 nL) were fabricated to simulate cloud droplet-relevant sizes. Freezing properties of Snomax®, illite NX, nanocrystalline cellulose (NCC), and Alaskan soil samples were examined to reproduce previous laboratory results with microliter freezing assays within marginal uncertainties for different droplet volumes. Results indicated consistency in the highest freezing temperature and efficiency of Snomax® as well as the lowest freezing temperature and efficiency of NCC for both techniques. Positive controls with known suspension samples were established, affirming the microfluidic device's reliability. The microfluidic device demonstrated an INP detection limit per unit mass of 10<sup>5</sup> to 10<sup>13</sup> per gram over the temperature range of 5 to 35°C, verifying its applicability to atmospherically relevant freezing conditions and providing accurate data for parameterization development. Lastly, the tools and approaches developed in this work are intended to be integrated into science teaching at a primarily undergraduate Hispanic-serving institute, contributing to disseminating knowledge and fostering a deeper understanding of ice nucleation processes among students.

### Environment-Microbiome-Plant Interactions Drive Root Microbiome Assembly Outcomes and Impact Conifer and Shrub Seedling Performance in Post Wildfire Soils

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Temperate conifer forests are faced with unparalleled challenges from anthropogenic climate change. Rising temperatures contribute to increasing frequency of wildfire, and prolonged drought can result in shifts from forest-toshrub-dominated ecosystem states. However, few studies explore ecoevolutionary hypotheses to predict how soil and root microbiome attributes shape the growth and drought tolerance of conifer and shrub seedlings, two traits that are critical to early competitive dynamics during revegetation after fire. In a greenhouse, researchers grew Grand fir (Abies grandis) and Snowbrush (Ceanothus velutinus) with live soil inocula from native conifer forests after various numbers of recent, high-severity wildfires (zero, one, and three wildfires within 25 years), with and without a drought treatment. The team used plant performance data and amplicon sequencing (16S, ITS, 18S) of root microbiomes to test predictions of how root microbiome attributes, such as guild abundance, microbial network connectivity, and the source of inocula, influenced early conifer and shrub seedling performance. Researchers hypothesized that environment-microbiome-plant interactions would play a key role in driving root microbiome outcomes and plant performance. The team found that root microbiomes from soils that experienced very different recent fire impacts had contrasting effects on root microbiome community assembly after one year of growth and soil microbiomes from different sites resulted in contrasting effects on seedling growth. The proportions of mutualistic and pathogenic fungi predicted stronger and weaker growth for Grand fir, respectively, but not for Snowbrush. Bacterial pathogens had a negative effect on the growth of Snowbrush, but only under drought conditions. Root microbiomes with greater fungal network connectivity were associated with stronger plant performance. This study shows that changes in microbiome assembly processes can impact microbiome function and may translate into changes in seedling performance in post-wildfire soils.

#### Virtual

### Pinpointing the Unlikeliness of Ida's New York City Hourly Intensity: Climate Change, Non-Stationarity, and Extreme Precipitation

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The remnants of Hurricane Ida caused major damage and loss of life in the northeastern United States on September 1, 2021. Over 40 people died in the storm across the United States, 11 of whom died in flooded basement apartments within New York City. The storm was so catastrophic because the maximum hourly precipitation intensity, recorded as 3.47 inches at Central Park, was unprecedentedly high for the region. The team contextualizes this storm's unprecedented nature within the historical record and projects its risk in terms of likeliness of occurrence and consequences in the near- to medium-term future using stationary and nonstationary hazard analyses techniques. The project shows that there is a multifold increase in the expected future risk when nonstationary models conditioned on future temperature projections are used as opposed to stationary models that assume no climate change. These results can be translated to potential future damage costs to the city by planning for events that would be expected under climate change. The results also reinforce the pressing need for improved urban stormwater management systems that can handle higher intensity rainfall as climate change continues to impact the weather and subsequently urban cosmos.

#### Virtual

### Effects of Global Warming and Elevated Carbon Dioxide on Peatland Ecosystem Productivity and Greenhouse Gas Emissions: A Modeling Study

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https://www.tnstate.edu/doe-rdpp

Peatlands are important ecosystems storing more than 20% of the global soil carbon. However, the impacts of global warming and elevated atmospheric carbon dioxide  $(CO_2)$ concentration on peatland ecosystem productivity and soil greenhouse gas [GHG, such as  $CO_2$ , methane (CH<sub>4</sub>), and nitrous oxide  $(N_2O)$ ] remain unclear. In this study, researchers simulated the dynamics and controls of peatland soil CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O emissions using a process-based model (Forest Denitrification-Decomposition; Forest-DNDC) under different temperature and CO<sub>2</sub> conditions. The simulations were based on the long-term DOE Spruce and Peatland Response Under Changing Environments (SPRUCE) experimental study where spruce peatland ecosystems were exposed under five temperature levels (i.e., +0, +2.25, +4.5, +6.75,  $+9^{\circ}$ C) and CO<sub>2</sub> conditions (+0, +500 parts per million). Data measured at the experimental plots from 2015 to 2021 were used to drive and parameterize the DNDC model. Preliminary results showed strong seasonal and interannual variations of net ecosystem exchange (NEE) of CO<sub>2</sub> and GHG, especially soil CO<sub>2</sub> and CH<sub>4</sub>. Both CO<sub>2</sub> and CH<sub>4</sub> emissions increased with temperature increase. With global warming, NEE shifted from carbon sink to source. Elevated CO<sub>2</sub> had limited impacts on NEE and GHG emissions. Results of this study could improve understanding of the magnitudes and controls of peatland productivity and soil GHG emissions.

### Advancements in Urban Heat Island Dynamics: Integrating Remote Sensing and Ground-Based Measurements

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The Urban Heat Island (UHI) phenomenon continues to pose significant environmental challenges in urban areas, exacerbating heat-related health issues. Building upon the previous work on the urban surface energy budget and land surface temperature (LST), this study presents novel insights into the dynamics of UHI and its impacts on urban environments. Researchers leveraged a combination of remote sensing satellite observations and ground-based measurements, including flux towers, Unmanned Aerial Vehicles (UAVs), infrared cameras, and handheld devices. Advancements were made in downscaling LST data, achieving a 5-minute temporal and 30-meter spatial resolution over New York City (NYC). Furthermore, collaboration with Brookhaven National Laboratory (BNL) under the DOE Research Development and Partnership Pilot (RDPP) facilitated community field data collection in Manhattan and Brooklyn, engaging local communities in understanding UHI's health and societal impacts. The team's recent study extends these efforts by analyzing the relationship between air and surface temperatures in urban settings from 2002 to 2022. Data were sourced from Automated Surface Observing Systems (ASOS), the New York Urban Hydro-Meteorological Testbed (NY-uHMT), and high school student collections. Analysis of 227 ASOS stations worldwide revealed discrepancies between air and surface temperatures, particularly notable in urban areas during summer. Field campaigns conducted in the summer of 2023 yielded crucial data, underscoring the heterogeneity of land-surface temperatures at a microscale level, a detail not captured by satellite data such as NASA's MODIS. The results demonstrated a weaker correlation between air and surface temperatures in urban settings, emphasizing the complex nature of UHI. The findings highlight the critical need for urban land-cover mitigation strategies, such as green infrastructure and reflective roofing, to combat the effects of extreme heat waves. This research contributes significantly to the understanding of UHI dynamics, providing a foundation for future urban planning and public health initiatives.

### Evaluating the Impact of Hydrologic Variability and Land Use on Stream Ecosystem Health in the Piedmont Region

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Land use and land cover change have strong impacts on aquatic metabolism in streams and rivers through changes in hydrologic regimes, light, nutrients, and other factors. However, efforts to quantify these relationships are difficult because of the disparate and convolved impact multiple changes can have on metabolism. This study utilizes a comprehensive dataset of stream metabolism modeled from dissolved oxygen from 2008 to 2021 across 11 sites in the Piedmont region of the U.S. southeast to investigate the response of aquatic ecosystems to fluctuations in hydrology, using resistance and resilience as key indicators. Resistance is defined as the degree to which production and respiration rates are altered by flow events, while resilience measures the time required for these rates to revert to their baseline levels following such events. The analysis further incorporates watershed land-use characteristics and a riparian vegetation index to categorize each site providing insights into the interplay between watershed characteristics and stream ecosystem health. This study is expected to reveal the dynamic responses of stream metabolism to fluctuating hydrologic conditions with a particular focus on how varying watershed characteristics and the presence of riparian vegetation might influence these interactions.

### Evolution of Moist Static Energy During Madden-Julian Oscillation Using Tropical Western Pacific Atmospheric Radiation Measurement Observations

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The evolution of moist static energy (MSE) is intimately associated with the organization and propagation of the Madden-Julian oscillation (MJO). Past studies on MJOassociated MSE, for the most part, were confined to the open ocean or large tropical islands and relied primarily on reanalysis data or model simulations. This research team presents a systematic analysis of the intraseasonal variation in MSE in the tropical western Pacific (TWP) using longterm, high-quality, ground-based observations from two Department of Energy Atmospheric Radiation Measurement (DOE-ARM) sites located over small islands: Manus and Nauru. Researchers use 14 years (2000 to 2014) of value-added radiosonde and microwave radiometer products, and researchers routinely measured surface meteorological variables to estimate vertical profiles of MSE during MJO propagation across the western Pacific. The team used large-scale precipitation tracking to identify MJO propagation (instead of usual MJO tracking using Realtime Multivariate MJO; RMM) since it can provide the exact location of the MJO precipitation centroid (unlike the RMM index). Therefore, composites of MSE vertical structure can be developed as a function of the location of the MIO precipitation centroid, and the distance between the ARM sites and the MJO. The results show (1) the humidity dominates the MSE profiles during active MJO phases, while temperature plays a role in suppressed and transition phases; (2) the mid-tropospheric moistening from the transition to active phases is consistent with the moisture-mode theory; and (3) MJO events propagating closer to the TWP-ARM stations show an abrupt increase in MSE at the beginning of active phases instead of a gradual increase in MSE seen in the composites of all MJO events. This result may reconcile the differences found in past studies that differ from each other related to slow and fast evolution in MSE in the TWP.

### Examining Microbial Respiration and Chemical Signatures of Urban Rivers Differing in Flow History

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Intermittent rivers and ephemeral streams (IRES) comprise up to 60% of the total length of all river networks on the globe. Due to both climate change impacts and water abstraction, stream intermittency is predicted to become more widespread in the future. Water and sediment chemistry in IRES may differ from perennial streams due to the occurrence of hot spots or hot moments of biogeochemical activity caused by drying and rewetting of streambed sediments in IRES. This project examines how stream water and sediment chemistry in intermittent and perennial stream reaches differ spatially in the San Antonio River (SAR) watershed, which is located in the metropolitan area of San Antonio, TX. This work is in collaboration with staff scientists at Pacific Northwest National Laboratory and is, in part, using protocols developed by the Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems consortium to gain a mechanistic understanding of organic matter recalcitrance and quantity across streams with varying flow history. Initial results indicate variable dissolved organic carbon (DOC) and total nitrogen (TN) concentrations across sites in the SAR watershed. During dry periods, intermittently flowing sites generally yield greater DOC (9.7  $\pm$  3.3 mg L<sup>-1</sup>) but lower TN (1.2  $\pm$  0.5) than perennial (DOC:  $6.7 \pm 0.9$ , TN:  $7.1 \pm 5.0 \text{ mg L}^{-1}$ ). This effect is likely due to perennial sites having baseflow maintained by high N-sourced water such as treated wastewater or impounded reservoirs with fertilizer runoff. Identification of specific microbial taxa via amplicon-gene sequencing (16S rRNA) in variable flow streams are in progress. Additionally, wet-season sampling and targeted in situ respiration measurements of candidate intermittent and perennial sites are planned for 2024.

### Late Additions

### WATERSHED SCIENCES UNIVERSITY PROJECT

### Virtual

### Feedback Loops and Abiotic Determinants of Biomass Growth and its Impact on Chromium Reduction in the Hyporheic Zone

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Within the hyporheic zone, a complex interplay of abiotic processes dictates the growth conditions of biomass. Factors like soil heterogeneity, stream conditions, temperature fluctuations, and nutrient availability all converge to shape this environment. Given the hyporheic zone's potential to bioremediate contaminants through biotic and abiotic reduction, decoding these growth determinants has broader ecological significance. In this study, the team presents a numerical exploration of how varied initial conditions influence biomass growth and its impact on modeling of chromium reduction through Monod kinetics. The modeling approach simulates a two-dimensional cross-section of the hyporheic zone, integrating surface water-groundwater interactions through river stage changes. To effectively capture bioclogging dynamics and soil respiration, researchers enhanced the reactive transport model, PFLOTRAN, to account for biomass decay influenced by fluid velocity and the dependency of biomass growth on temperature. The diverse simulation conditions, augmented by sensitivity analyses for pivotal abiotic factors, offer holistic insights into microbial growth dynamics and chromium reduction through PCA and correlation heatmaps. Comprehensive comparisons of mean values over time, and spatial variability distributions of key parameters, serve as the foundation of the analysis. In addition to investigation of correlated features in the simulations, researchers also present a deep-learning-based upscaling model. The team tested 5x and 10x upscaling and showed that the method offers accuracy and considerable speed up compared to Monte-Carlo simulations. The team investigated the nuanced relationships between abiotic elements and bacterial proliferation and highlight how these relationships impact chromium reduction in the hyporheic zone. Through this multifaceted study, the team offers a fresh perspective on the modeling of reactive transport in the hyporheic zone.

### **TERRESTRIAL ECOLOGY UNIVERSITY PROJECT**

### Eddy Covariance of Methane in Upland and Seasonally Flooded Forests in the Amazon Basin, Working Towards the Contribution of Tree Stems on Ecosystem Methane Fluxes

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Methane emissions from tree stems have been gathering much attention (Barba et al. 2019; Pangala et al. 2017). However, in seasonally flooded (várzea) forests along the Amazon River, researchers have only scant measurements of the dynamics of tree stem emissions. The team is developing seasonal ecosystem and component methane flux measurements in both a várzea and an upland forest near Santarém, Brazil. The team will present preliminary eddy covariance and monthly tree and soil flux results from the upland tower site and a seasonally flooded site. These initial measurements were made as part of the measurement systems' development and testing and the várzea forest site selection process. All discrete fluxes will be analyzed using the gasfluxes R package, which was modified to work the flux measurement data gathering methods. Eddy covariance analysis will be conducted with the openeddy R package.

Methane stem fluxes in the upland site appear to be higher in tree species with lower wood density and higher sap flux rates. Seasonal variability of stem fluxes in the upland forest is very small, suggesting that the source methane variability is much lower than in várzea forests. Várzea tree stem fluxes are several orders of magnitude higher in the wet (flooded) season relative to the dry season and the upland forest site. Tree stem flux measurements along vertical profiles show an exponential decay of methane emissions with height, and most methane is emitted within the first 2 m of height along the stem. Cylindrical diffusion of methane flux along tree stems best fits the measured flux data from the várzea forest sites.

Barba, J., et al. 2019. "Methane Emissions from Tree Stems: A New Frontier in the Global Carbon Cycle," *New Phytologist* **222**(1), 18–28. DOI:10.1111/nph.15582.

Pangala, S. R., et al. 2017. "Large Emissions from Floodplain Trees Close the Amazon Methane Budget," *Nature* **552**, 230–34. DOI:10.1038/nature24639.

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