



2023 ENVIRONMENTAL SYSTEM SCIENCE PI MEETING ABSTRACTS

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



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Bethesda, MD

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

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2023 Environmental System Science PI Meeting Abstracts



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TERRESTRIAL ECOLOGY

University Projects

Measuring and Modeling Methane Emissions at the Coastal Terrestrial-Aquatic Interface

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Incorporating the coastal terrestrial-aquatic interface (TAI) into Earth systems models requires a better mechanistic understanding of the biogeochemical processes that regulate greenhouse gas emissions, including methane (CH₄). In 2021, researchers started a model-experiment (ModEx) project to address some of these knowledge gaps that includes automated measurements of CH₄ emissions in a coastal wetland, a mesocosm warming × salinity × flooding experiment, and updates to the TAI configuration of PFLOTRAN.

The network of 12 automated chambers in Smithsonian's Global Change Research Wetland has been operating continuously since April 2021, with soil heating added in February 2022. The high frequency of these flux measurements mean that researchers can look at responses to drivers that are both cyclical (diurnal, tidal) or stochastic (heat waves, storm events). Researchers found that CH₄ emissions are higher from warmer, wetter soils, as expected, but also that emissions are consistently higher at night than during the day, regardless of environmental conditions.

Using these field data, researchers were able to update the PFLOTRAN configuration to incorporate periodic hydrological cycling, including diurnal cycles. While previous simulations did not alter plant-mediated transport to account for respiration at night, researchers were able to use the empirical data to incorporate the simultaneous effects of day/night and tides, allowing the model to match the dynamic the team captured in the autochamber measurements. Using this updated model structure, researchers found that the indirect effects of environmental stress on vegetation can produce greater shifts in biogeochemical processing capacity than the direct effects on biogeochemical processes.

The mesocosm experiment was designed to understand some of these underlying mechanisms, by including pots with and without vegetation at two sites of differing salinity. As expected, vegetated pots from the freshwater marsh released about 10 times more CH₄ than vegetated pots at the brackish marsh and about 10 to 100 times more CH₄ than bare pots at both sites. Surprisingly, sea level rise and

warming increased CH₄ emissions from the brackish site but had minimal to no impact on CH₄ emissions from the freshwater site. These relationships are either a function of carbon limitation at the freshwater marsh or of mechanistic differences in CH₄ production and consumption between the sites, both of which researchers will investigate.

Virtual

Dynamic Root Foraging and Allocation in E3SM: Exploring Responses and Feedbacks at Four United States AmeriFlux Sites

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Future climate projections predict extreme weather events, such as hurricanes and drought, will increase in frequency and duration over the coming century. These climate changes will stress natural vegetation that are adapted to current climate conditions. Forests respond to stress by allocating resources to where they are most needed, by redistributing fine roots deeper into the soil during times of drought and altering allocation between above and belowground components. These stress responses are not present in many modern Earth System Models, reducing the ability to predict ecosystem responses to stress and how said responses will affect future climate. Here, researchers utilize E3SM in default mode, but also with the addition of two stress dynamics, a dynamic rooting depth module where plants can forage for water and nitrogen, and a dynamic allocation subroutine, allowing redistribution of resources between above and belowground components. Firstly, researchers examined root dynamics globally, and found that by allowing roots to forage, the timetable of recovery from stress events is altered differentially between dry and humid ecosystems. Researchers then use point scale simulations in four forest AmeriFlux sites with long observation records paired with tree ring data, Morgan Monroe State Forest (US-MMS), Missouri Ozarks (US-MOz), and Sylvania Wilderness (US-Syv), and Niwot Ridge (US-NR1). Researchers simulated all four sites in default mode, with dynamic rooting depth, dynamic allocation, and the combination thereof. While there are some small changes in response to rooting depth, E3SM was completely agnostic to the presence or absence of fine root biomass. As such the dynamic allocation subroutine reduced allocation to fine roots by a factor of 10 in some cases.

Currently, there is no function for fine root biomass in E3SM and closely related models, therefore any stress events

that might alter allocation to roots is likely misrepresented in E3SM climate projections and may result in an overestimation of future productivity. Ideally, fine root biomass should have a function, such as nutrient and water absorption in such models. Fine roots are extremely difficult to study *in situ*; therefore, modeling root dynamics are required to develop hypotheses about how changes to root systems will impact ecosystems and the climate. Future work should focus on adding this functionality to E3SM based on observations of fine roots.

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, while the winter snowpack is shrinking and soil freeze/thaw events are increasing in high latitude ecosystems. The severe thermal impact of soil freeze/thaw cycles in winter, coupled with warming during the growing season, reduces soil carbon (C) cycling, but increases nitrogen (N) and phosphorus (P) cycling in soil. Nevertheless, the root and microbial mechanisms leading to these shifts are unclear. Researchers hypothesize that under climate change across seasons, microbes and plants exhibit a trade-off between stress metabolism and soil C, N, and P uptake (short-term) and biomass production (longer-term) that scales up to impact C and nutrient export at the watershed-level. To test this hypothesis, researchers are conducting a model-data integration study using the Climate Change Across Seasons Experiment (CCASE) at the Hubbard Brook Experimental Forest (HBEF) and a plot-to-watershed-level biogeochemistry model, PnET-BGC. At CCASE, replicate field plots receive one of three climate treatments: growing season warming (+5 °C above ambient), warming + freeze/thaw cycles (+5 °C above ambient in growing season plus up to four freeze/thaw cycles in winter), and reference conditions (no treatment). Researchers have found that warming + freeze/thaw cycles induce redox stress and select for anaerobic N cycling microbes, while potentially shifting the majority of microbial C-cycling activity from organic to deeper mineral soil horizons during winter. Soil microbes are also evolving under these

conditions to increase decomposition of plant and soil C, but decrease decomposition of organic P, potentially decoupling C, N, and P outputs to associated aquatic ecosystems both temporally and spatially. This research couples isotopic tracer experiments through soils and roots at CCASE with soil metagenomic, metatranscriptomic, and metaproteomic data, as well as new high-throughput characterizations of trait and gene evolution in individual soil bacteria and fungi to reconstruct evolution of potential plant and microbial C, N, and P metabolism at CCASE over the past decade. Researchers plan to incorporate immediate and evolved responses of microbial C, N, and P cycling into new versions of PnET-BGC, including an evolutionary algorithm applied to specific C, N and P flux calculations. This research tests the conceptual understanding of plant and microbial physiology responses to severe, compounding soil temperature perturbations across seasons, as well as the utility of a forest stand-level manipulative climate change experiment to understand the biogeochemical dynamics of a forest watershed undergoing rapid environmental change.

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

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Nitrogen (N) deposition has enhanced carbon (C) storage in temperate forest soils. However, it remains unclear whether this soil C will persist as N deposition declines across the region. Given that this uncertainty directly impedes the ability of predictive models to project future soil C stocks, there is a critical need to determine how N-induced shifts in key microbial traits drive soil C stabilization. To address this uncertainty, the team's objectives are to (1) quantify variations in taxon-specific and community-level microbial traits across gradients in microbial community composition, the distribution of ectomycorrhizal (ECM) and arbuscular mycorrhizal (AM) trees, and N availability; and (2) integrate this data into a novel predictive framework that enhances the ability to project the regional soil C consequences of N deposition in temperate forests.

Under ambient N, researchers found that decomposition pathways in AM soils have greater flexibility in which

microbes are the active decomposers and what they produce than those in ECM soils. Under elevated N, researchers found evidence of a reduction in functional evenness for both mycorrhizal types with a narrowing of the distribution of active taxa taking up C and N. However, when researchers examined how N fertilization impacts the response of microbes to simulated root exudation, there were greater declines in function and growth in AM soils than ECM soils. The maintenance of function in ECM soils appeared to result from elevated N promoting the activity of certain bacterial phyla at the expense of others. These empirical results have been instrumental in improving the soil decomposition model that represents microbial groups based on substrate preference. The model was able to capture increases in soil C in response to N fertilization when the team reduced the competitive advantage of microbes that degrade complex C. Upon cessation of N fertilization, the model showed that the added soil C was highly susceptible to loss under increasing temperature. Coupled together, the experimental and model results highlight that integrating microbial traits into models alters predictions of the response of soil C in temperate forests to global change.

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. 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, making the OM vulnerable to microbial attack. Carbon dioxide (CO₂) can then be released, and nutrients can be moved back into rapidly cycling pools. Because rhizodeposits from living roots are complex mixes of compounds, and their quality and quantity are known to vary with environmental conditions, this study conducted two greenhouse and growth chamber experiments exploring whether live root systems mobilize MAOM off minerals as a function of (1) altered morphology and physiology triggered by Barley Yellow Dwarf Virus (BYDV) and (2) low soil nutrient and water availability.

Also being examined are the interactive effects of mycorrhizal infection and BYDV infection on plant physiology, soil solution DOM, and association of OM with ferrihydrite.

BYDV attacks many grasses, often reducing root:shoot and making roots “sticky” with organic compounds. Researchers added labeled MAOM (¹³C-glucose bound to ferrihydrite) to soil prior to planting *Avena sativa* (oats) either infected or uninfected with BYDV. Among other results, respiration from soil under infected plants had a higher percent ¹³C-MAOM-derived CO₂ (p = 0.001), but a similar total amount of MAOM-derived CO₂ was respired from whole pots planted with infected and uninfected plants.

To investigate nutrient and water limitations, researchers tested the individual and interactive effects of nitrogen (N), phosphorus (P), and water limitations on the fate of ¹³C-labeled MAOM added to soil then planted with oats. Overall, total MAOM mineralization was strongly correlated with root biomass, and drought-reduced MAOM mineralization. P limitation intensified MAOM mineralization most during initial plant growth stages; N limitations spurred enhanced MAOM mineralization during later growth stages.

To examine mycorrhizal infection and BYDV infection, researchers grew oats in sand with mycorrhizal symbiont inoculum (*Rhizofagus irregularis*, formerly *Glomus intraradicis*) or with *R. irregularis* and BYDV infection. Analyses are ongoing. To date, results indicate shoot biomass predicts the number of mycorrhizal vesicles per cm of root, and the extent of extra-radical hyphae is best predicted by root branching frequency and crown biomass. Analysis is underway of mycorrhizosphere contributions of OM that can become associated with ferrihydrite in soil.

Using the *ecosys* modeling program, researchers are exploring the system-scale implications of altered kinetics of binding of OM to minerals and altered capacity for OM binding in 16 grasslands and 7 forests.

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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Peat soils are major terrestrial carbon stores and large natural producers of biogenic greenhouse gases (i.e., methane and

carbon dioxide). These gases accumulate in the soil matrix to be subsequently released to the atmosphere, therefore directly influencing climate change. While recent advances have been made with regards to the prediction of carbon fluxes, many uncertainties still exist to properly understand the spatial distribution of hot spots and hot moments for the accumulation and release of biogenic gases. This can be attributed to the limitations in terms of effective noninvasive methods that can be deployed at scales of measurement relevant for the imaging and identification of such hot spots.

This project has been testing a prototype ground-penetrating radar (GPR) unit (the Geodrone 80 from Mala) mounted on a small unoccupied aircraft system (sUAS) to efficiently identify the presence of hot spots and hot moments in subtropical peat soils of the Everglades and explore how certain physical (i.e., soil structure) and biochemical properties (i.e., metabolic pathway) may influence its dynamics. Delays with drone acquisition and study site selection due to changes in drone legislation in Florida initially shifted efforts to laboratory simulations, where a set of high frequency antennas were suspended over a peat monolith (extracted from the Water Conservation Area, WCA1 in the Everglades) using a custom-made rail system that allowed for the antenna to move autonomously (simulating airborne measurements using a drone) that were able to successfully monitor changes in dielectric permittivity associated with biogenic gas build up and release over a period of several months. At the field scale, an initial set of drone measurements using Mala's 80 MHz Geodrone were collected from two locations in the WCA2, Everglades. At each of these two locations, Geodrone flights were programmed to collect data in a grid over an approximate 100 m² area. These preliminary airborne results via the Geodrone show promise for generating maps of static gas content distribution across the peat column as based on changes in EM wave travel time when peat thickness is known (or assumed constant over specific areas). Furthermore, these measurements will be expanded into time-lapse mode in order to define temporal changes in EM wave travel time across the peat column associated with the build-up and release of biogenic gases that will allow researchers to efficiently isolate the presence of hot spots for gas accumulation and release.

Reduced Sensitivity of Carbon and Water Exchange to Soil Moisture in Temperate Trees Exposed to Chronic Throughfall Removal

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Climatic change is projected to alter precipitation patterns and increase the risk of drought in substantial portions of Earth's temperate biomes. Responses of plants to longer-term shifts in precipitation may have consequences for both short- and long-term land-atmosphere feedbacks, mediated by changes in rates of carbon and water exchange under a given set of environmental conditions. Here, researchers investigated the influence of long-term throughfall reduction on: (1) diel and seasonal rates of transpiration, canopy conductance, and gross primary productivity; (2) responses of these processes to environmental conditions, including soil moisture; and (3) relationships of these processes with soil and atmospheric moisture during short-term natural dry periods. Using a 3-year throughfall exclusion experiment in U.S. central hardwood forest, researchers examined co-occurring species responses to reduced precipitation and soil water availability by quantifying physiological process rates of three tree species under ambient rainfall, moderate (-45%), and severe (-80%) throughfall removal. The results show that throughfall removal alters tree species' relationships between shallow soil moisture and processes such as transpiration, canopy conductance, and gross primary productivity. During dry periods, transpiration, canopy conductance, and gross primary productivity slow down at any given soil moisture level and/or are less responsive to fluctuations in soil moisture. Thus, under future climatic conditions, drier growing seasons would decrease productivity at a given level of soil moisture, depending on species' plasticity in physiological traits.

Student

Environmental Controls on Local Thaw of a Vegetation-Protected Permafrost Plateau

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Atmospheric temperatures in the Northern Hemisphere have warmed faster than the global average, and this

amplified warming is expected to strengthen in the future. Trends in permafrost temperature are consistent with trends in atmospheric temperature, with widespread observed warming. However, other environmental factors, such as ecologic, hydrologic, and topographic conditions, also regulate permafrost temperature, progression, and stability. Vegetation-protected permafrost, located in regions with a MAAT above 0°C, persist in these unfavorable climates due to favorable ecologic conditions. Understanding how this vegetation-protected permafrost degrades is crucial, because vegetation-protected permafrost acts as a forecaster and predictor of thaw in more northern latitudes.

To better understand environmental factors affecting soil temperature and permafrost progression in the vegetation-protected zone, the team instrumented a rapidly degrading permafrost plateau in the western Kenai Peninsula lowlands of south-central Alaska. Researchers paired high-resolution soil temperature data with a suite of observed environmental variables across a topographically and vegetatively diverse area. This site is located at the warm southern fringe of the permafrost zone.

During the study, all locations but those with the highest relative-elevation and canopy density thawed rapidly. The stability of these topographically high locations was due to both vegetation and topographic protection. Low relative elevation locations thawed rapidly due to not having these protections, while moderate relative elevation locations, which shared many protections with high relative elevation locations, thawed rapidly due to their vulnerability to rain-induced warming and thaw. Additionally, the team observed an abrupt increase in average annual thaw rates during the duration of our study (2020-2022) compared to the time since the last study at the site (2015-2020). The study period contained the three snowiest years and three of the four wettest years since 2015. These snowy and wet years caused thaw-inducing environmental controls to be amplified, which caused a fourfold increase in thaw rates. As northern high latitudes continue to become warmer and wetter, and more of the permafrost zone experiences MAATs above 0°C, we may see similar environmental controls on permafrost progression across more of the permafrost region.

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

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Methane (CH₄) 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 CH₄ budgets. The project objectives are: (1) to improve the understanding of the controls on CH₄ fluxes in forested mineral soil wetlands; and (2) to better understand the effects of landscape position and forest composition on the CH₄ fluxes between terrestrial ecosystems and the atmosphere. Using a coupled modeling-experimental approach, researchers started measuring the spatial and temporal dynamics of CH₄ fluxes in soils and woody structures (stems and knees) of temperate bald cypress (*Taxodium distichum*) and other bottomland hardwood stands and incorporating the measurements into a land surface model to improve the model representation and predictions of CH₄ fluxes. Soil collars and custom-built chambers were installed in the stems and knees of trees along eight sites that span a hydrologic gradient from the terrace to the stream channel in Western Kentucky's Clarks River National Wildlife Refuge (CRNWR). Results showed that the Cherry Bark Oak (*Quercus stellate*) stand was a greater soil CH₄ sink (-1.47 ± 0.60 nmol/m²/s) than a nearby Bald cypress stand (-0.44 ± 0.35 nmol/m²/s).

The team found significant differences in soil CH₄ fluxes (p-value < 0.02) between stand species composition (p-value < 0.02; *T. distichum* vs. rest of species, and *Q. stellate* vs. *Quercus pagoda*), but no significant differences in stem CH₄ fluxes among species (p-value = 0.25). Contrary to some studies, researchers found no significant difference among CH₄ fluxes across stem heights. There were significant differences among stem and soil fluxes (*T. distichum*: p-value = 0.01, *Acer rubrum* + *Liquidambar styraciflua*: p-value < 0.001). Soils took up CH₄, while stems emitted CH₄. The results showed higher average soil CH₄ uptake rate in high knee density areas compared to no knee areas (p = 0.004) that can offset the observed knees CH₄ emission. Researchers will use ongoing monitoring to improve the understanding of soil-vegetation interaction in hardwood bottomland wetlands and incorporate these functions into ongoing land surface modeling efforts.

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

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Mycorrhizal fungi provide plants with nutrients in return for photosynthate, linking above- and belowground processes. Forests dominated by arbuscular (AM) versus ectomycorrhizal (EcM) fungi have well-documented differences in their distributions of soil carbon (C) and nitrogen (N). However, the mechanisms driving these patterns are uncertain.

Potential mechanisms include differences in leaf litter quality, rhizodeposition, fungal nutrient acquisition strategies, and fungal necromass quality. The observations across forests of the Eastern U.S. indicate that fungal nutrient acquisition strategies are likely driving these patterns. Researchers found that as the relative abundance of EcM fungi with the ability to produce peroxidases increased, the proportion of soil organic matter that was mineral-associated decreased. Researchers developed a mycorrhizal fungi-explicit version of the Carbon, Organisms, Rhizosphere, and Protection in the Soil Environment model called Myco-CORPSE wherein EcM fungi can mine soil organic matter for N, but AM fungi cannot. Using the model, researchers found that EcM fungi with a strong ability to mine N from the slow and necromass organic matter pools could induce saprotrophic N limitation and thus increase the amount of soil organic matter in the unprotected pool. This effect was strongest in cold ecosystems with more recalcitrant plant litter inputs. To experimentally test how litter quality versus fungal traits affect soil organic matter, researchers are currently incubating six different types of dual ¹³C and ¹⁵N-labeled litter in soil mesocosms at forests in New Hampshire, Illinois, and Georgia where each have six plots differing in the abundance and dominant family of EcM-associated trees. Lastly, to investigate the role of rhizodeposition, the team carried out a greenhouse experiment wherein eight species of seedlings (four AM and four EcM) were grown in a ¹³C-labeled atmosphere under three levels of N fertilization. Over one growing season, rhizodeposition was greater from EcM seedlings than AM seedlings and increased with increasing N availability in EcM but not in AM seedlings. Despite these differences, the net effect of the seedlings on soil carbon was similar across mycorrhizal types implying increases in

rhizodeposition were balanced by increases in decomposition. This ongoing research is bringing new insights into the mechanisms driving mycorrhizal differences in soil organic matter cycling that researchers are incorporating into regional simulations of Myco-CORPSE.

Student

Investigating the Potential of Airborne Ground-Penetrating Radar (GPR) to Identify Hot Spots for Biogenic Gas Accumulation and Release in Peat Soils from the Everglades

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Subtropical peatlands play a vital role in the global carbon budget by generating fluxes of biogenic gases mainly composed of methane and carbon dioxide. Previous studies during the last 2 decades have advanced understanding on how to predict these carbon fluxes at a variety of spatial and temporal scales in peat soils; however, the spatial variability of gas accumulation (i.e., hot spots) at the matrix level is still unclear, mostly due to the difficulties of noninvasively imaging these areas. While most studies have traditionally relied on point measurements (i.e., flux chambers) or methods like eddy covariance with large footprints that may lack the resolution to properly capture hot spots for gas accumulation and release, several studies have shown the potential of ground-penetrating radar (GPR) to noninvasively image gas distribution at the matrix scale. However, the method still relies on ground-based measurements that are time consuming and limited in coverage. In this study, researchers tested the potential of airborne GPR measurements to efficiently characterize gas distribution in peat soils and identify the presence of hot spots at the laboratory scale. This study represents a first step before deploying field-based GPR measurements from a small unoccupied aircraft system (sUAS). A high-frequency antenna was suspended over a large peat monolith (0.75 m x 0.31 m x 0.25 m, extracted from the Loxahatchee Impounded Landscape Assessment in Water Conservation Area 1, FL, using a custom-made rail system that allowed for the antenna to move autonomously and monitor changes in dielectric permittivity associated with biogenic gas build up and release at high temporal resolution. Airborne GPR measurements were combined with transmission GPR, gas traps with time-lapse cameras (to infer gas fluxes), and gas chromatography (to analyze gas composition). Preliminary results show the potential of airborne GPR measurements to isolate hot spots for gas accumulation in peat soils at the laboratory scale and thus show

promise for the use of sUAS at the field scale to characterize hot spots more efficiently for gas accumulation and release in the Everglades.

Hydraulic Redistribution in Forests: Spatial and Temporal Drivers of Variation and Consequences for Climate Feedbacks

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The Earth system models used for climate projections are still limited in their ability to accurately simulate observed soil moisture and its control on transpiration and photosynthesis. One reason for this may be that these models do not realistically represent a process known as hydraulic redistribution (HR), where roots transport water from wet to dry soils. To better inform these models, this project seeks to: (1) understand drivers of spatial and temporal variation in rates of HR across the landscape; (2) pilot the implementation and realistic parameterizations of these drivers in models; and (3) test the new parameterizations against observations to better understand the consequences of their inclusion for climate feedbacks. Researchers plan to: (1) quantify the prevalence and magnitude of HR across tree species, tree sizes, and drought durations in mixed temperate forest species with contrasting hydraulic strategies by measuring soil and plant hydrologic/hydraulic properties and fluxes; (2) use stable isotope techniques to trace the origins of water sources in the soil and in water fluxes within the potentially lifting trees; and (3) compare the field data to model simulations to help improve model realism. Most studies of HR to date have focused on vegetation in arid to semi-arid regions or coniferous species where water is limited either annually or seasonally. The study sites are located in Indiana, a humid region where droughts historically are episodic events.

Climate projections, however, 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. This provokes the question: to what extent does HR alleviate water stress and contribute to maintaining photosynthesis rates during droughts? Researchers will use experiments to quantify the prevalence and magnitude of HR to test parameterizations in two models that couple with the E3SM

Land Model (ELM): (1) FATES-HYDRO, a plant hydrodynamics model that builds on the FATES model by adding multiple plant hydraulic traits linked to vegetation dynamics and carbon/water fluxes; and (2) ELM with a new plant hydraulic stress (PHS) representation. A key difference between these models is that FATES-HYDRO, unlike ELM-PHS, considers plant water storage, which may affect the partitioning of water to plant storage vs. HR.

Experimentally Determined Traits Shape Bacterial Community Composition 1 and 5 Years Following Wildfire

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Wildfires represent major ecological disturbances, burning 2% to 3% of the Earth's terrestrial area each year with sometimes drastic effects on above- and belowground communities. Soil bacteria offer an ideal, yet understudied system within which to explore fundamental principles of fire ecology due to their vast diversity and critical ecological functions, such as organic matter mineralization. To understand how wildfires restructure soil bacterial communities and alter their functioning, the team sought to translate aboveground fire ecology to belowground systems by determining: (1) which microbial traits are important post-fire; and (2) whether changes in bacterial communities post-fire affect carbon (C) cycling. Researchers employed an uncommon approach to assigning bacterial traits by first running three separate laboratory experiments in which they directly determined which microbes survive fires, grow quickly post-fire, or thrive in the post-fire environment, while also tracking carbon dioxide emissions. Then, to evaluate the importance of each trait in structuring soil bacterial communities, the team quantified the abundance of taxa assigned to each trait in a large field dataset of soils 1 and 5 years after wildfires of varying burn severities in a globally important ecosystem—the boreal forest of northern Canada. First, analogously to fire-adapted plants, fast-growing bacteria were found to rapidly dominate post-fire soils, but, in contrast to their larger counterparts, they return to preburn relative abundances between 1 and 5 years post-fire. Although both fire survival and an affinity for the post-fire environment were statistically significant predictors of post-fire community composition, neither was particularly influential. These results suggest that uncharacterized factors, such as vegetation recovery or bacterial dispersal, may be more

important for determining community composition over decadal timescales. Second, results indicate that soil C fluxes post-wildfire are not likely limited by the microbial community, suggesting strong functional resilience. From these findings, the team offers a traits-based framework of bacterial responses to wildfire, which could be of broad use to researchers seeking to understand interactions between C cycling, bacterial communities, and disturbance, while the integrated experimental-field observational approach could be translated and applied to many different systems. For subsequent experiments, researchers have returned to the region and are investigating how wildfires may change microbial C use efficiency, using both glucose and pine wood as substrates. In addition, the team is determining whether incorporating laboratory-identified traits into a biogeochemical model improves predictions of C mineralization post-fire.

Student

Simulated Burn Impact on Soil Properties and Carbon Cycling

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Boreal forests hold a massive terrestrial reservoir of carbon (C), which is held both above- and belowground. Wildfire in the boreal forest can drive changes in quantity and composition of C held in the soil via heat-induced tree mortality and production of coarse woody debris at the soil surface, incomplete combustion of organic matter leading to production of pyrogenic organic matter, and volatilization and loss of C to the atmosphere. To understand how wildfires impact soil C cycling and how this may vary with burn severity, the team aims to determine the impact of burning and burn duration on soil properties, including pH, total C, and total nitrogen (N), and on C cycling in the weeks to months post-burn. Researchers collected soil cores from twelve sites across Wood Buffalo National Park, Alberta, Canada and allowed cores to air-dry to simulate drought conditions. Cores from each site were subjected to burn simulations in a cone calorimeter for either 30 s or 120 s or were kept as controls and not burned (N=4 for each treatment). Soil carbon dioxide efflux was measured daily using an automated sampling system connected to a cavity ring-down spectroscopy instrument for 10 weeks post-burn. The team fit a two-pool decay model to respiration curves to estimate changes in the fractional size and decomposition

rates of fast- and slow-cycling C pools. The simulated burns altered both soil C and N stocks, driving shifts in C:N ratios. These changes were accompanied by immediate increases in soil pH, with larger effects in soil cores subjected to the longer burn duration. During the 10 weeks post-burn, overall respiration rates (per gram dry soil) were lower in burned vs. unburned soil. These results suggest that the immediate impact of burning on soil C and the soil environment may drive a slowdown in C cycling in the weeks following fire, and this effect may be larger with increasing burn durations, which may be related to increasing burn severity in the field. Next steps include linking changes in C cycling to changes in bacterial and fungal community composition and microbial C use efficiency post-fire.

Greenhouse Gas Emission and Redox Potential in Biochar- and Compost-Amended Urban Soil Under Contrasting Water Saturation Conditions

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Soils are significant sources and sinks for greenhouse gases (GHGs) such as carbon dioxide (CO₂), methane (CH₄) and nitrous oxide (N₂O). There have been many studies investigating GHG dynamics in agricultural soils but there have been limited studies for urban soils. This project was designed to investigate urban soil GHG emissions affected by soil hydrologic conditions, organic soil amendments (biochar and/or compost), and redox chemistry through soil mesocosm experiment. The soil material was a compost-soil blend that is sold from the City of McAllen, TX, representing a typical urban gardening soil. The soil was packed into a total of 12 columns (5-gallon buckets) at a bulk density of 1.1 g cm⁻³. The treatment consisted of four amendment treatments for biochar, compost, biochar + compost, and no amendment as control) and the amendments were surface-applied at 5-cm thickness. Grass sod (Saint Augustine) was placed on the top of the amendment with surface application of 14-14-14 (N-P-K) fertilizer. The amendments were considered as subplots and each subplot will receive repeated wetting-drying cycle at full saturation, half-saturation, or unsaturated condition up to 8 weeks. For instance, the full-saturation treatment will be held for the first 2 weeks and will be drained for the next 2 weeks (unsaturated) and this 4-week cycle will be repeated twice. Each soil column will be instrumented with redox probes (SWAP

instrument, Inc., Netherland) that measures redox potential (Eh in milli-volt) by 10-cm increment. Soil moisture will be measured manually using a commercial soil moisture probe (up to 15 cm deep). GHG measurements will be done through LI-COR soil gas flux survey chamber equipped with CO₂/CH₄ trace gas analyzer (LI-7810) and N₂O trace gas analyzer (LI-7820). Currently, preliminary testing for redox probes under various water table conditions and background GHG emission measurements are in progress. The presentation will present the first-round of soil mesocosm experiment results along with physicochemical characterization of the amendments and soil material.

The Promise of Microwave Remote Sensing for Understanding Dryland Carbon-Water Dynamics

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Dryland ecosystems occupy ~40% of Earth's land surface and exert an outsized role in shaping global carbon and water cycling. Unfortunately, dryland ecosystems are notoriously difficult to study at broad scales, due to their large spatial and temporal heterogeneity. As such, fundamental ecological questions remain unresolved in drylands. For example, what is the role of atmospheric drivers versus soil moisture in controlling carbon-water fluxes? And which soil moisture pools (shallow versus deep) matter the most for ecosystem function? To assess these questions, researchers synthesized gross primary productivity (GPP) and evapotranspiration (ET) data from all eddy covariance towers located in American drylands, most of which contained soil moisture depth profiles. Researchers found that GPP and ET were most sensitive to fluctuations in shallow soil moisture and varied only slightly in response to other drivers such as vapor pressure deficit, temperature, and light. Researchers then assessed the ability of land surface models to properly capture this dynamic by comparing the soil moisture sensitivity of *in situ* ecosystem fluxes to output from 15 CMIP6 models. The team found that these models significantly underestimated the sensitivity of GPP to soil moisture fluctuations and overestimated the sensitivity of ET. Finally, the team evaluated the degree to which six different l-band and x-band microwave remote sensing products

could accurately capture fluctuations in GPP and ET and found that they were tightly linked to ecosystem fluxes on a daily timescale. The significant ability of these products to capture dryland fluxes at a high frequency was due to the fact that they generally tracked soil moisture dynamics. The results indicate that microwave remote sensing products show great promise for capturing the dynamics of dryland ecosystem function and suggest that assimilation of these data into existing land surface models may improve simulations of dryland fluxes.

Student

Increasing Signature of Old Carbon in Headwater Streams Following 14 Years of Permafrost Thaw

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<http://www2.nau.edu/schuurlab-p/GIPEHR.html>

Soils in the permafrost regions comprise only 15% of the global soil area yet contain an estimated 33% of global soil carbon. These soils have accumulated almost three times the amount of carbon currently in the atmosphere as a result of limited microbial decomposition and water flow in subzero conditions. However, recent analyses indicate that the Arctic is warming at more than twice the rate of the global average and that there is an accelerated decomposition and export of ancient permafrost as this soil thaws. Though permafrost organic carbon has often been viewed as less decomposable, with deeper, older layers containing more recalcitrant carbon, the vulnerability of stored soil carbon to release is quite variable and dependent on inherent differences in the decomposability of individual molecules and changes to the landscape.

Increasing atmospheric release has been well-documented for decades; however, streams are more difficult to monitor, and thus, their role in the Arctic carbon cycle has often been overlooked. This study assessed the contribution that Arctic headwaters play in long-term permafrost carbon release at the Arctic Carbon and Climate (ACCLIMATE) observatory, located in the discontinuous permafrost zone of interior Alaska. Researchers compared the age of carbon exported vertically, through respiration of carbon dioxide with that exported laterally, as dissolved organic carbon (DOC) over 18 years. Age was estimated using radiocarbon (¹⁴C) dating. The team found that both vertical and lateral signals follow similar release patterns, releasing large, ancient pulses of permafrost carbon at the same time. This indicates that

landscape-level permafrost degradation signals can be tracked contemporaneously both in streams and the atmosphere. Further, it was found that permafrost carbon contributions to both ecosystem respiration and DOC fluxes have increased over 14 years as changing ecosystem conditions increasingly favored permafrost carbon release. However, the contribution of permafrost carbon has increased three times more quickly within DOC fluxes than it has within ecosystem respiration fluxes (22‰ year⁻¹ $\Delta^{14}\text{C}$ of DOC vs. 6.5‰ year⁻¹ $\Delta^{14}\text{C}$ of ecosystem respiration), highlighting the emerging importance of headwaters in the export of ancient, permafrost-derived carbon. Overall, whether the release of permafrost carbon be terrestrially derived or aquatic, this increase in ancient carbon release signifies that permafrost systems in this region are destabilizing as a result of an accelerating climate change feedback.

Student

Modeling Methane Dynamics in a Bottomland Hardwood Wetland

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Climate and environmental changes have a significant effect on wetlands, making it urgent to accurately model their methane (CH₄) dynamics. There have been limited attempts in modeling the fluxes and pathways of CH₄ dynamics in bottomland hardwood forested wetlands. This research study aims to improve the representation of wetland CH₄ dynamics by incorporating emissions from temperate bald cypress (*Taxodium distichum*) trees and their knees—woody structures that form above the root of the bald cypress—in the CH₄ modeling systems.

The Peatland Ecosystem Photosynthesis Respiration and Methane Transport (PEPRMT) model is a process-based biogeochemical model designed to estimate wetland carbon dioxide and CH₄ fluxes (Oikawa et al. 2017). Currently, the team is modifying this model to represent methane release from the bottomland hardwood wetland ecosystem. Data from five eddy covariance flux towers representing upland and bottomland hardwood and forested wetland sites from different parts of the United States and data from cypress

swamps owned by Murray State University, KY, are being arranged to fit into the model. Researchers are customizing the model to incorporate emissions from bald cypress knees into the model's carbon/methane cycle. The model will then be validated at the flux sites. This improved representation and understanding of methane dynamics will increase the accuracy of the assessment of methane releases from woody wetland ecosystems in their current state and provide better knowledge for future climate change scenarios.

Oikawa, P. Y., et al. 2017. "Evaluation of a Hierarchy of Models Reveals Importance of Substrate Limitation for Predicting Carbon Dioxide and Methane Exchange in Restored Wetlands," *Journal of Geophysical Research: Biogeosciences* **122**(1), 145–67.

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

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Global change is affecting terrestrial ecosystems in multiple ways. In mountain ecosystems, direct effects (i.e., raised soil temperatures) and indirect effects (i.e., early snowmelt, decrease in snowpack) of warming are co-occurring. The ability to forecast belowground responses to these complex global change drivers has been hindered by a lack of long-term studies. Yet, these belowground studies are vital as soil fungi are key decomposers in terrestrial ecosystems, potentially flipping soils from carbon sinks to carbon sources. Here researchers examined soil fungal responses (composition and abundance) to a 29-year-long warming experiment and a 4-year-long early snowmelt manipulation at the Rocky Mountain Biological Laboratory in Gothic, CO in 2019 to 2021. The team used complementary approaches by pairing experimental data with those collected the same year from nearby environmental gradients in temperature (i.e., elevation) and snowmelt date (i.e., at different slopes and aspects). Environmental gradients capture long-term ecological and

evolutionary variation but can be confounded by many covarying abiotic and biotic factors. Experiments allow researchers to understand the role of a specific global change driver but may not occur over long enough time periods to capture both ecological and evolutionary responses.

Soil fungal communities varied substantially in response to abiotic environmental gradients. Up to 8% of the variation in fungal composition was explained by elevation (a long-term proxy for temperature) and 15% of variation in fungal composition was explained by aspect (a long-term proxy for snowmelt date). Snowmelt date in the collection year explained an additional 10% of variation in fungal composition. Experimental treatments affected fungal communities less.

Experimental early snowmelt explained 6% of the variation in fungal communities whereas warming only explained 4% of the variation in fungal communities. Fungal abundance followed similar trends with hyphal lengths varying the most by elevation and aspect and the least in experimental manipulations. Overall, the results suggest that fungi are more sensitive to historical and contemporary snowmelt date (which varies by 56 days since 1975) than the direct effects of warming per se. Because fungal response to snowmelt is strong, and snowpack and melt dates are highly variable, future ecosystem models may be improved by including fungal functions across the transition in snow cover. Future research in the group is focused on comparing plant, fungal, and biogeochemical phenology in response to snowmelt date.

Virtual

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

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High-latitude regions are warming faster than the rest of the planet, increasing plant trait variation across local to regional scales. Due to the critical role plant traits (i.e., leaf nitrogen, leaf phosphorus, specific leaf area) have on gross primary production and plant and soil respiration, understanding the spatial patterns of trait variability across rapidly changing tundra ecosystems is essential for improving the performance of carbon cycle processes in Earth System Models. The project aims to improve the representation of above-ground and belowground traits in models by characterizing

directly observable plant functional traits from remotely sensed data, and predict nonobservable (i.e., belowground) traits by leveraging trait-environment relationships and trait covariation. This trait information will be integrated into the Terrestrial Ecosystem Model (TEM) to quantify and predict regional carbon (C) balance in the Alaskan tundra.

In the summers of 2021 and 2022, the team established eight sites representing dominant plant community types in northern Alaska. To date, five of the eight sites were sampled (remaining sites will be sampled in 2024); four located within the taiga-tundra ecotone and one on the Arctic Coastal Plain. In each site, researchers measured species percent cover, canopy height, and edaphic parameters, and collected leaf samples and root cores to characterize traits at the species, functional type, and community levels. In addition, each site was imaged using hyperspectral and light detection and ranging (LiDAR) sensors onboard an uncrewed aerial system (UAS). UAS-derived plant trait mapping are found to well-represent ground-based observations of leaf area, specific leaf area, and biomass (additional leaf and root traits are currently being processed), explaining between 65 to 95% of the overall trait variability at each site. Site-specific trait maps and models were used to evaluate regional upscaling assumptions and methods using overlapping 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 the understanding of high-latitude carbon-climate feedbacks.

Impacts of Hydraulic Redistribution on Root Exudation and Rhizosphere Biogeochemistry

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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. In this project, researchers are using greenhouse experiments to quantify how HR impacts the quantity, timing and location of root exudation in two temperate hardwood tree species. The results from these experiments are used to parameterize a root-scale biogeochemical model and a plant-scale ecohydrological model that will permit researchers to examine the effects of HR-driven exudation on rhizosphere microbial activity.

Initial 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. Researchers have developed a workflow that allows imaging of root exudation using anodic aluminum oxide as a blotting medium to transfer exudates from the root-soil system in a spatially preserved manner. Analysis by FT-ICR-MSI confirmed that a broad suite of exudates can be analyzed in this manner. In upcoming work, researchers will apply this method to roots that are experiencing both HR and non-HR conditions to identify how HR changes the flux of exudates at the root scale.

Initial modeling work on this project has focused on expanding the TREES ecohydrological model to include subroutines for root exudation, including variable exudate fluxes based on user-defined parameters and variable C:N stoichiometry of exudate fluxes. Future work will focus on incorporating experimental data into this model, using measured root architectures to scale from individual root observations to whole-plant exudate fluxes.

Production Phenology of Fine Roots and Ectomycorrhizal Hyphae Are Closely Linked but Vary Across Monospecific Stands of Temperate Tree Species

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The production of fine roots and mycorrhizal fungi together account for between 15 and 45% of annual productivity in forest ecosystems though these estimates are highly uncertain. The root-fungal synergy is responsible for acquisition of water and nutrients heterogeneously distributed throughout the soil profile and sporadically available in pulses of

availability throughout the year. Given the high cost to construct and maintain roots and mycorrhizal fungi, and the variability in resource availability, the timing of root and fungal production plays an important role in determining the effectiveness and efficiency of belowground resource acquisition.

However, little is known about the timing of belowground production, especially fungal production, and how fungal phenology varies with tree hosts. In this study, the team used *in situ* minirhizotron imaging to characterize the timing of fine root production and the production of fungal hyphae and rhizomorphs in 10 monospecific forestry plots, each dominated by either an angiosperm or gymnosperm tree host that associates with ectomycorrhizal fungi. Images were collected at The Morton Arboretum in Northern Illinois for 3 years (2019 to 2021) that encompassed both relatively wet years (2019 and 2020) and a relatively dry year (2021).

Both roots and mycorrhizal fungi showed strong seasonality in their production. Across years, root production typically peaked around July to August (most angiosperms) to September (most gymnosperms). Production of fungal hyphae peaked shortly after peaks in root production, typically in late September to October. The similar timing and strongly positive correlation between root and fungal production echoes the close relationship between the two partners.

However, it is important to note that compared to the variation in root production observed across different tree species, and between angiosperm and gymnosperm hosts in general, the timing of peak fungal production was more consistent across all plots indicating that environmental conditions were also important. Water in particular, known to be important for fungal growth in general, appeared to be an important factor controlling fungal production across years. Peak fungal production in 2019 was roughly a month earlier than peak production in 2020. This is consistent with strong fall wetting events that occurred roughly 1 month earlier in 2019 compared to 2020. Fungal production overall was strongly reduced in 2021 compared to 2019 and 2020, with 2021 being the notably drier year. Future work will link patterns of fine root and fungal phenology to leaf phenology and environmental conditions and enable accurate parameterization of belowground phenology in Earth system models.

Student

Impact of Watershed Hydrologic, Thermal, and Nutrient Inputs on Wetland Methane Emissions in Subarctic Bogs

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Methane, a potent greenhouse gas, accounts for a large portion of the global warming potential of permafrost thaw. This is particularly true in areas with ice-rich permafrost. When ice-rich permafrost thaws, the ground subsides, creating thermokarst features such as thaw bogs. These bog systems are the topographically lowest points of their surrounding landscape and therefore receive and collect runoff from the surrounding permafrost-underlain watershed. This hydrologic connection between bog systems and their surrounding watersheds can amplify bog methane emissions through the transport of thermal energy and nutrients into the bog complex.

Data previously collected by the research team showed warm rain early in the growing season can advect heat into wetland soils from the surrounding watershed. This thermal input increased wetland soil temperatures and in turn significantly increased methane emissions by supporting microbial and vegetative processes. These results highlight how the watershed–bog connection can influence methane. Currently, the ability of inputs from the permafrost plateau to affect biogeochemical processes is not recognized in field studies nor implemented in models.

This project is advancing understanding of the watershed–bog connection and clarifying the conditions in which inputs from the permafrost plateau affect land–atmospheric exchange of carbon. The team continues to increase understanding through field observations at a well-instrumented bog complex in interior Alaska and pair these observations with Earth system modeling done by project collaborators. Recently installed field equipment allows the research team to track hydrologic, thermal, and nutrient inputs across the permafrost plateau and throughout the bog complex. This data is then paired with observed methane fluxes to better understand watershed–bog dynamics and the resulting methane emissions.

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

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The strength of Earth System Model (ESM) projections of ecosystem responses to climate change hinges upon robust modeling of biomes that differ widely in climate sensitivity. Drylands, covering more than 40% of the terrestrial surface, strongly influence the trend and year-to-year variability in global sink strength. Yet, the seasonality and magnitude of biogeochemical processes in drylands are challenging to represent in ESMs, partly because capturing plant-available water dynamics and/or ecosystem functional responses to plant-available water is difficult. Plant-mediated hydraulic redistribution (HR; water movement via plant roots between soil compartments that differ in water potential) offers a major avenue for improving the representation of dryland soil moisture dynamics. This project tests the idea that soil moisture dynamics and ecosystem function in dryland biomes cannot be well understood or modeled without a better representation of HR. To improve the representation of HR in ESMs, researchers are coupling point measurements of sap flow and soil moisture, with ecosystem-scale measurements of NEE, GPP, and Re, and the use of the data assimilation approach to develop the Terrestrial Ecosystem (TECO) model to address three objectives:

- (1) identify the key mechanisms determining the presence and magnitude of HR in species/biomes across a range of semi-arid western woodlands/forests;
- (2) quantify seasonal patterns of HR across dryland species and biomes to determine when HR has the biggest impact on soil moisture dynamics and the mechanisms driving them, and;
- (3) scale plant-level patterns in HR to ecosystem-level NEE, GPP and Re in response to precipitation anomalies.

Researchers use parallel measurements of HR in dominant species in the fetch of AmeriFlux towers in three key biomes (ponderosa pine forest, piñon-juniper woodland, and juniper savanna) that vary in elevation, climate, and deep soil moisture availability. Researchers supplement existing instrumentation to measure root sap flow and soil water potential revealing the timing/magnitude of HR in each dominant species (Objective 1). Researchers measure the timing of HR and the local and ecosystem conditions under

which it is observed (Objective 2). Researchers use these data and the flux tower record (2009 to present) for data assimilation to improve model structures and parameterization in TECO to provide important advances in the ability of ESMs to capture HR and predict dryland ecosystem function. Finally, researchers compare tree-level measurements of HR with measurements of ecosystem function to correlate the HR patterns associated with variation in GPP, Re, and NEE using empirical data for comparison with the TECO-HR model (Objective 3).

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 storage. These growth forms respond differently to variation in climate and resource availability, and their responses to future climate change are poorly understood. The overarching objectives of this project are to carry out an observational campaign to advance the understanding of liana traits and strategies, develop a liana-enabled forest dynamics model that leverages the observations, and to engage with the Earth System Modeling (ESM) community to plan for the eventual inclusion of lianas into ESMs. Here, researchers report on four activities, which have brought researchers closer to meeting these objectives. (1) Researchers have measured liana traits and conducted meta-analysis of liana trait data. On average, researchers find marked differences between lianas and trees in terms of their hydraulic traits and xylem anatomical traits. They also identified significant variation in hydraulic traits across liana species. (2) Researchers incorporated these results into a mechanistic but simple model of liana-tree couplet 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) Researchers measured tree growth and liana colonization status of over 1,700 trees at a study site in Guanacaste, Costa Rica. They found that the number of colonized trees is increasing and that heavily infested trees have lower relative growth rates than other trees. Liana

colonization also impacted the relationship between tree growth and rainfall. (4) Researchers incorporated lianas into the TROLL forest dynamics model and developed new schemes for leaf production and turnover. TROLL represents the three-dimensional canopies of trees and lianas, discretized into 1 m³ voxels. Thus, for a given host tree canopy, the scheme specifies where it is that lianas prefer to grow new leaves. Researchers have carried out a sensitivity analysis and tested the model's ability to simulate observed patterns. (5) Researchers have implemented liana-enabled forest dynamics in TROLL. These dynamics include the ability of lianas to colonize an arbitrary number of trees in its neighborhood and the ability of trees to shed lianas.

Virtual, Early Career

Biogenic and Abiotic Processes Impacting Reactive Nitrogen Oxide Fluxes to and from Soil

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Nitrogen (N) cycle processes play a crucial role in regulating the overall abundance of oxidized inorganic nitrogen in terrestrial ecosystems and are responsible for initiating the subsequent loss of soil N via volatilization and leaching. This poster will outline the laboratory's effort to understand the sources and sinks of reactive nitrogen oxides (nitric oxide, nitrogen dioxide, nitrous acid) with the ultimate goal of improving how fluxes of reactive nitrogen oxides are represented in chemical-transport models. This presentation will share results of field campaigns aimed at studying the impact of vegetation on reactive nitrogen oxide emissions from soil, in addition to the contribution of freshly senesced leaves in the autumn. Researchers found that plants compete with microbes for nutrients, which has an important impact on modulation of released gases. In addition, the leaves of some deciduous tree species become sources of nitric oxide in forested regions when nitrogen that is not reabsorbed during senescence is released to the atmosphere. This research was enabled by the development of a new catalyst capable of allowing measurement of nitric oxide, nitrogen dioxide, and nitrous acid in real time in both the field and laboratory setting. Implications for atmospheric chemistry will be discussed.

Virtual

Nonstructural Carbohydrate Depletion Impairs Ponderosa Pine Water Relations in the Field

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Ongoing climate change is increasing the frequency and intensity of hot droughts in many forested regions across the globe. These conditions lead to progressive dehydration, which often pushes trees over critical physiological thresholds (e.g., permanent turgor loss, hydraulic failure, and cell death), leading to increased mortality rates. However, predicting when, where, and which trees will die of drought remains a challenge in part because interdependent processes leading to drought-induced mortality are not fully understood. Although loss of water transport capacity (hydraulic failure) is pervasive across dead trees and considered the driver of tree death, it remains unclear whether other processes during dehydration may contribute to hydraulic failure. In greenhouse experiments, stored nonstructural carbohydrates (NSC) have been shown to affect osmoregulation and turgor maintenance, which could in turn affect soil–plant–atmosphere hydraulic function. However, whether NSC depletion impairs osmoregulation in trees in the field has not been tested.

Here, researchers tested whether NSC availability influences water relations in naturally occurring ponderosa pine saplings. Trees receiving ambient levels of precipitation or experimental drought were subjected to either full sun or to 8 weeks of shade-induced NSC depletion. The team measured NSC content in needles, along with predawn needle water potential, osmotic potential, and turgor pressure prior to shading and at weekly intervals during the NSC-depletion treatment. Preliminary results indicate higher NSC content in drought trees relative to nondrought trees, likely due to cessation of growth at the onset of drought. Shading reduced NSC content in needles under both ambient precipitation and experimental drought. Drought trees exhibited lower total and osmotic potential (more negative) than trees under ambient precipitation. As summer drought intensified, osmotic potential in trees under ambient light decreased regardless of drought treatment. In contrast, in shaded trees, osmotic potential remained constant, indicating that the depletion of NSC decreased osmoregulation capacity and turgor maintenance.

This work provides first tentative evidence demonstrating that NSC availability mediates water relations in naturally

occurring trees in the field—both under natural precipitation and imposed drought stress. More generally, results suggest that under recurring or prolonged droughts, as is expected with ongoing climate change, consumption of NSC may predispose individuals to increased vulnerability to drought. Therefore, accounting for variation in NSC pools and their influence on water relations among individuals and species may improve predictions of drought-induced mortality risk.

Ecosystem and Soil Respiration Radiocarbon Detects Old Carbon Release as a Fingerprint of Permafrost Destabilization with Climate Change

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www2.nau.edu/schuurlab-p/

Permafrost has accumulated organic carbon in cold and waterlogged soils over thousands of years and now contains three times as much carbon as the atmosphere. Global warming is degrading permafrost with the potential to accelerate climate change as increased microbial decomposition releases soil carbon as greenhouse gases.

A 19-year time series of soil and ecosystem respiration radiocarbon from Alaska provides long-term insight into changing permafrost carbon dynamics in a warmer world. Nine percent of ecosystem respiration and 23% of soil respiration observations had radiocarbon values more than 50% lower than the atmospheric value. Furthermore, the overall trend of ecosystem and soil respiration radiocarbon values through time decreased more than atmospheric radiocarbon values did, indicating that old carbon degradation was enhanced.

Boosted regression tree analyses showed that temperature and moisture environmental variables had the largest relative influence on lower radiocarbon values. This suggested that old carbon degradation was controlled by permafrost thaw and soil drying together, as waterlogged soil conditions could protect soil carbon from microbial decomposition even when thawed. Overall, changing conditions increasingly favored the release of old carbon, which is a definitive

fingerprint of an accelerating feedback to climate change as a consequence of permafrost destabilization.

Simulating Greenhouse Gas Fluxes Across the Terrestrial–Aquatic Interface: A Spatially Explicit Approach

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

Terrestrial–aquatic interfaces (TAIs) undergo frequent variations in soil saturation that result in heterogeneous distribution of greenhouse gas (GHG)–regulating components—such as dissolved organic carbon content, terminal electron acceptor (TEA) availability, pH, and nutrient abundance. The formation of soil microsites (i.e., microscale regions with unique biogeochemical characteristics compared to the surrounding area) enable seemingly disparate processes—such as oxic respiration and methanogenesis—to occur simultaneously within one soil column. Most GHG flux models fail to predict such co-occurrences as they assume a homogeneous distribution of GHG–regulating components across a given soil column. Here, the project addresses this discrepancy by developing a spatially explicit model of GHG fluxes in TAIs. To mimic *in situ* conditions, researchers conduct incubations of intact soil cores collected from a hydrology gradient in Old Woman Creek, OH, near Lake Erie, which the team subjects to hydrological fluctuation. High-resolution two-dimensional maps of dioxygen concentration are obtained using colorimetric planar oxygen optode imaging. Spatially specific measurements of pH and redox state are obtained using microelectrodes, and dissolved nutrient/TEA abundances are obtained from extracted porewater samples. GHG fluxes are measured continuously using a Cavity Ring-Down Spectrophotometer (Picarro G2508). These measurements are used to generate probability distribution (or density) functions of GHG–regulating components. By employing a model-experiment framework and constraining a spatially explicit GHG flux model (DAMM-GHG) coupled with a redox-reactive network module (AquaMEND), the project assesses whether

capturing redox heterogeneity in soil microsites aids with improved predictions of GHG fluxes from TAIs.

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

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The overall research project goal is to assess how co-occurring drought and deluge climate extremes will impact key carbon (C)–cycling processes known to be important for carbon–climate feedbacks. The team will address this goal via research in the 280,000 km² 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 carbon dioxide sink. The key hypothesis being tested is that when a compound climate perturbation of an extreme deluge occurs 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 are planning to conduct a field experiment designed to quantify the magnitude of C-cycling responses to drought and deluge events (independently and combined) and identify the underlying mechanisms resulting in positive drought–deluge interactions that can lead to hot moments of C cycling. Both above- and belowground C-cycle responses to climate extremes will be quantified during this 3-year experiment. To scale up from the plot-level experiment to the shortgrass steppe ecoregion, the team will use historical climate data to quantify the regional frequency of potential drought–deluge interactions and remote sensing products (e.g., normalized difference vegetation index 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, extreme drought, deluge, and drought-deluge perturbations will be simulated 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 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.

Acclimation of Photosynthesis and Respiration in Tropical Plants at the TRACE Site Under Long-Term Experimental Warming and Hurricane Disturbance Recovery

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<https://www.forestwarming.org/>

Background and Methods. Climate change projections over the next 80 years predict increased global temperatures and more frequent and intense hurricane disturbances. How plants respond to these changes could have huge implications for how carbon is cycled between ecosystems and the atmosphere. Thermal acclimation, or the ability of individuals to change metabolic processes to work more efficiently at different temperatures, could help plants perform better at higher temperatures or mitigate the effects of temperature damage. While thermal acclimation has been observed in temperate systems, it could be minimal to nonexistent in tropical systems that experience narrower temperature ranges than temperate systems. The team assessed the acclimation potential of plant physiological processes to experimental warming and tracked their changes during post-hurricane recovery at the Tropical Responses to Altered Climate Experiment (TRACE), a long-term *in situ* experimental warming project in eastern Puerto Rico where the forest understory is warmed +4°C above ambient temperature using infrared heaters. Researchers measured temperature response curves on root respiration, leaf photosynthesis and respiration, and leaf thermotolerance for experimentally warmed and ambient temperature

plants; these data were collected after two major hurricanes impacted the study site in 2017.

Results and Conclusions. Tropical root respiration did not acclimate through changes in root specific respiration rates, but ecosystem root respiration declined under warming due to lower root biomass. Hurricane disturbance increased variability in root respiration, but the effects are likely short term. Researchers observed photosynthetic thermal acclimation through wider thermal niche breadth but at the cost of overall lower photosynthesis for warmed plants. Additionally, photosynthesis was highest after the hurricanes and decreased as the canopy closed. The temperature optimum for photosynthesis, which did not show signs of acclimation, was near the temperature of warmed plots. Leaf respiration was not affected by experimental warming but decreased with canopy closure after the hurricanes. Leaf thermotolerance did not acclimate to warming and was lowest when the canopy was open and increased as the canopy closed. Together, these results suggest that there is a brief boost to understory carbon assimilation after hurricane disturbance independent of warming effects but at the potential cost of higher respiration. Scaling these responses to an ecosystem is dependent on overall biomass of the system and environmental forcings. Future goals are to estimate the biomass at the site and model the carbon flux responses to experimental warming using the E3SM Land Model–FATES model.

Variation in Methane Emissions from Tree Stems in Upland and Seasonally Flooded Forests in the Amazon Basin

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Methane emissions of tree stems have been gathering much attention (Pangala et al. 2017; Barba et al. 2019); however, in seasonally flooded (várzea) forests along the Amazon River, researchers have only scant measurements of the dynamics of 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 stem flux measurements from specific tree stems in the seasonally flooded sites. These initial measurements have been made as part of the measurement systems'

development and testing and the várzea forest site selection process. All fluxes will be analyzed using gasfluxes R package, which the team modified to work R scripts for flux measurement data gathering methods.

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 the 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, suggesting that 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.

STEEP-CF: Storm Treatment Effects on Ecosystem Processes of Coastal Forests

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Coastal forests and other coastal ecosystems are influenced by complex hydro-biogeochemical processes, which are heavily impacted by climate change. Increased frequency and intensity of storm events and sea level rise (SLR), already occurring and predicted to accelerate due to climate change, affect biogeochemical processes that ultimately shape ecosystem resiliency and can push these ecosystems into an alternative stable state. This project aims to improve understanding and predictive capacity of ecosystem changes, feedbacks, and subsequent responses to different types of flood disturbances in coastal forests. This project takes advantage of DOE-funded TEMPEST (Terrestrial Ecosystem Manipulation to Probe the Effects of Storm Treatments), a large-scale manipulation experiment that has been established (but treatments have not started) to test flood disturbances of brackish and freshwater pulse events in a temperate coastal forest. Researchers will additionally provide a mechanistic understanding of the processes affected by these disturbance events by performing

controlled mesocosm experiments on large intact soil columns obtained from the field site, where flooding events can be carefully manipulated and monitored. This newly funded project will address four knowledge gaps: (1) feedbacks between hydrologic disturbance events and belowground processes; (2) mineral-mediated carbon release after flooding disturbances; (3) successive hydrologic disturbance impacts on soil carbon dioxide and methane flux magnitudes and metabolic pathways; and (4) limitations of soil biogeochemical models under flooding scenarios.

Sensitivity of Shrub–Grass Dynamics to Plant Hydraulics Under Drought in FATES and BiomeE

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Shrubs are encroaching upon and eradicating many grasslands across Earth. Researchers currently have limited understanding about why this is occurring and the resulting consequences for critical ecosystem services, such as carbon sequestration. This project is designed to address both of these knowledge gaps through a combination of observational, experimental, and process-based modeling approaches in tallgrass prairie of eastern Kansas. The team measured a wide range of above- and belowground morphological and physiological characteristics of shrubs and grasses, as well as soil carbon turnover rates within the grass–shrub ecotone. Researchers imposed a multiyear drought experiment to understand responses of grasses, shrubs, and carbon cycling to water stress. The team is incorporating this empirical understanding into process-based models to test hypotheses about why shrub encroachment is occurring and to project impacts of encroachment on ecosystem carbon storage. Some major findings from the project to date include: (1) shrub encroachment will likely increase under increased drought frequency global change scenarios. Researchers think this is because shrub species in this system have smaller yet more numerous conduits in roots, leading to more stable photosynthesis of shrubs during drought compared with herbaceous species; (2) increased atmospheric carbon dioxide (CO₂) may decrease the ability of fire to knock back shrubs because of

rapid colonization rates of shrubs under increased CO₂; and (3) Instead of the expected increases in carbon storage by shrubs in deeper soils, less carbon storage was found across all depths under shrubs due to lower root growth.

Here, the team focuses on the impact of droughts on shrub encroachment rates and will show results from benchmarking activities with long-term shrub/grass abundance data from Konza Prairie Biological Station and sensitivity analysis of shrub and grass plant functional types to various hydraulic parameters in two vegetation demographic models, FATES and BiomeE. These results provide mechanistic understanding of how shrub–grass boundaries may shift under various global change scenarios and identify areas where additional empirical understanding is needed.

Monitor and Constrain Tropical Ecosystem Sensitivity to Moisture (MACROCOSM) with Experimental Throughfall Exclusion in a Tropical Moist Forest

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Ecosystem sensitivity to water availability is pivotal to understanding resilience of tropical forests under a changing hydroclimatic regime. However, large knowledge gaps remain in how plants respond to moisture changes and how these responses in turn regulate ecosystem water dynamics, resulting in considerable uncertainty in ecohydrological predictions across state-of-the-art Earth system models. This project 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 Long-Term Ecological Research station, PR, where annual rainfall exceeds 3500 mm. Particularly, the team focuses 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 interpreting large-scale remote sensing observations and modeling long-term vegetation dynamics in the tropics.

At ecosystem scale, researchers combine state-of-the-art remote sensing techniques, especially microwave remote

sensing such as global navigation satellite systems–based vegetation optical depth measurement and ground-penetration radar, and soil moisture and water potential sensors at different depths to address the challenge. These new nondestructive measurements can continuously track subdaily patterns of both above- and belowground water dynamics and characterize fine-scale heterogeneity. At organism and tissue scale, the team monitors vegetation structural and hydraulic responses to drought by tracking leaf angle and canopy structure changes using terrestrial laser scanning and plant transpiration and root hydraulic redistribution using stem and root sap-flow sensors. Individual-level drought responses will be related to plant ecophysiological and hydraulic trait measurements available at the same site to quantify the role of canopy and roots in ecosystem sensitivity to moisture.

The team has finished the first field campaign, configured prototypes for *in situ* sensors, and started to collect pretreatment ecohydrological and forest structure data. The field data 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. Overall, the project is on track to develop an integrated, scale-aware, and predictive understanding of tropical ecosystem responses to hydroclimatic changes.

Virtual

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

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<https://biometeorology.umn.edu/research/quistococha-forest-reserve-qfr-amazonian-ameriflux-site-iquitos-peru>

Tropical peatlands play a significant role in the global carbon (C) budget. However, little is known about the biogeochemistry of these peatlands and in particular the C cycle processes and their responses to hydrometeorological

conditions. This leads to large uncertainties when constraining land surface models designed to forecast C budgets for tropical peatlands. This research made fundamental advances by providing the first ecosystem-scale carbon dioxide (CO₂) and methane (CH₄) flux observations in an Amazonian peatland and was the first to represent these systems within the E3SM Land Model (ELM) framework. Researchers found that the sink strength of natural palm swamp Amazonian peatlands is large but vulnerable to future warmer and drier conditions. Initial analyses of ecosystem-scale CO₂ and CH₄ fluxes showed the palm swamp peatland to be a large C sink (e.g., 440±187 g C m⁻² y⁻¹ in 2019). However, more recent data indicate that variations in hydrometeorological forcing can lead to a switch to a net C source. This change could be attributed to large scale climate variations, such as oscillations in La Niña/El Niño cycles. Field chamber observations showed unexpected subecosystem-scale C flux behavior, indicating complex partitioning of ecosystem-scale C emissions into soil and stem sources across seasons. Significant

seasonal variation was observed in soil and stem CO₂ fluxes (increasing during the dry season) and soil CH₄ fluxes (decreasing during the dry season). However, there were no significant differences in stem CH₄ fluxes between wet and dry seasons. Moreover, stem fluxes varied significantly among tree species and along their height profiles. Using these novel observations, the team improved ELM's ability to simulate CO₂ and CH₄ fluxes and the energy balance of tropical peatlands by advancing three tropical-specific biophysical functions and by using multiobjective parameter optimization. Global sensitivity analyses suggested strong control of parameters associated with vegetation photosynthetic activities. Further, the modeling assessments highlighted the knowledge gaps that need to be addressed in simulating tropical vegetation phenological physiology and the CH₄ transport from non-aerenchymatous tissues, such as stems. Subecosystem-scale and ecophysiological measurements are needed to characterize and develop

parameterizations of these processes to improve model capabilities and to advance ongoing modeling efforts to extend the C budget estimate to the Pastaza-Marañón foreland basin, which is the most extensive peatland complex in the Amazon basin.

Next-Generation Ecosystem Experiments

Basin-Scale Investigations of Topographic Influence on Permafrost Thaw in Ice Wedge Affected Landscapes

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<https://ngee-arctic.ornl.gov/>

In the past 30 years, climate change has resulted in a pronounced acceleration of pan-Arctic ice wedge degradation. In tundra settings, subsidence caused by the melting of ice wedges often drives profound changes in microtopography and surface hydrology. One common outcome from these changes is accelerated permafrost thaw beneath newly formed, meter-scale ponds known as thermokarst pools. Previous model-based investigations have predicted that, in some landscapes, the formation of thermokarst pools may accelerate the thaw of presently frozen soil organic carbon more than tenfold by 2100. However, field and satellite-based observations indicate that local trajectories of thermokarst pool formation, and hence the strength of these positive feedbacks, are highly variable and strongly influenced by environmental factors including macroscale topography. Researchers seek to quantify this variability by conducting basin-scale projections of permafrost thaw over next century in a variety of topographic settings. For this work, researchers apply the Advanced Terrestrial Simulator (ATS), a physics-rich integrated surface/subsurface hydrology code that has been specially configured to capture permafrost dynamics in ice wedge-affected terrain. Researchers focus on five landscapes in northern Alaska where rates of thermokarst pool expansion have been observed over the past 13 years using satellite remote sensing, allowing for model validation. The landscapes range from a coastal setting near Utqiagvik, AK, to the northern flanks of the Brooks Range mountains. Researchers designed the analysis to quantify how strongly variability in topographic setting

influences thaw-driven changes to surface inundation, and how strongly this variability in surface inundation impacts rates of future permafrost degradation. The research reduces a hitherto unaddressed source of uncertainty in regional projections of thaw in ice wedge-affected terrain. The results of this work will be used to improve the parameterization of inundation fraction within E3SM land models, such that the relationship between permafrost thaw and small pond formation will be modulated by macroscale topography. The new parameterization will enable pan-Arctic assessments of permafrost thaw to account for the influence of regional topography on local and highly variable trajectories of thermokarst pool evolution.

Virtual

Assessing the Transferability and Expandability of Random Forest Snow Distribution Models over Two Ngee-Arctic Study Sites

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Random forests are a flexible and interpretable machine-learning (ML) technique which have been used to model snow water equivalent at fine scales and to assess the drivers of snow distribution. Unlike “black box” ML techniques such as neural networks, decisions made by random forests can be traced back to splits along specific variables, making their decision-making process relatively transparent and allowing for the quantification of feature importance. However, previous work applying these approaches often focused on very small study domains, which raises questions regarding their transferability, expandability, and whether random forest feature importance can be used to draw conclusions about snow distribution drivers in broader areas, or if these results are very localized. Researchers test the random forest created by Bennett et al. (2022), modified to predict snow depth rather than snow water equivalent, on a broad expanse surrounding two field study sites (NGEE-Arctic Kougarak 64 Hillslope and Teller 27 watershed), and evaluated results against a 2022 LiDAR-derived snow depth product to better understand the expandability of the random forest model (NCALM 2022). Further, researchers trained the random forest model only on one Ngee site and tested on the other to evaluate the model’s performance across sites and over larger spatial scales outside of the training domain. Lastly, the team retrained the random forest model on the LiDAR data and examined the updated model’s feature importance and out-of-sample performance to see how these results

change when trained on a larger domain and with different training data. Ultimately, this assessment of random forest transferability provides context for other random forest snow distribution studies and can help inform future snow modeling efforts.

Bennett, K. et al. 2022. "End-of-Winter Snow Depth, Temperature, Density, and SWE Measurements at Teller Road Site, Seward Peninsula, Alaska," Data from 2019 Next Generation Ecosystem Experiments Arctic Data Collection. Accessed on February 24, 2022. DOI:10.5440/1798170.

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Bennett, K. et al. 2022. "End-of-Winter Snow Depth, Temperature, Density, and SWE Measurements at Kougarok Road Site, Seward Peninsula, Alaska," Data from 2022 Next Generation Ecosystem Experiments Arctic Data Collection. Accessed on February 24, 2022. DOI:10.5440/1888533.

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Wilson, C. et al. 2022. "End-of-Winter Snow Depth, Temperature, Density and SWE Measurements at Kougarok Road Site, Seward Peninsula, Alaska," Next Generation Ecosystem Experiments Arctic Data Collection. Accessed on February 24, 2022. DOI:10.5440/1593874.

Scaling from Species to Vegetation: NGEA-Arctic's Plant Functional Type Classification

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The Arctic system is highly sensitive to climate change, exerts key land-feedbacks relevant for global climate dynamics, and harbors a range of vegetation types comprised

of plant species with unique traits including mosses and lichens. For the future, a widespread redistribution of Arctic vegetation is predicted. Understanding and predicting how these redistributions affect climate is essential for reducing uncertainties in climate projections. Plant functional type (PFTs) provide a necessary framework for Earth system models (ESMs) to reduce the complexity of interactions between plants and their environment and predict vegetation responses to, and effects on, ecosystem processes.

PFTs represent a classification scheme between species and broad vegetation types based on shared similar characteristics (e.g., growth form) and roles (e.g., physiological property). An underlying assumption is that the functional role of vegetation can be identified by these linked sets of traits constrained by resources, based on the hypothesis of functional convergence. Researchers share: (1) the hierarchical classification scheme developed for use in the E3SM Land Model vegetation process modules as part of NGEA-Arctic phase three, including a crosswalk with the most common PFT classifications previously put forth for the Arctic; (2) methods to parameterize vegetation types and their PFTs; and (3) examples of remote sensing and modeling efforts in phase three that utilize the classification.

Estimating Permafrost Distribution, Soil Movement, and Their Controlling Factors in Arctic Environments Using Depth-Resolved Measurements of Resistivity, Temperature, and Deformation

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Discontinuous permafrost environments exhibit strong spatial heterogeneity and sharp transitions in soil and permafrost thermal conditions, subsurface hydrology, and carbon (C) and energy fluxes. This heterogeneity occurs at scales too small to be driven by weather forcing alone and is regulated by several mechanisms, some still poorly represented in Earth System Models though driving significant uncertainty in the trajectory of C fluxes. A better understanding of the permafrost conditions and soil movements, as well as their controls, is needed to improve the estimates of current and future soil C storage and release.

In this study, researchers investigate the soil deformation triggers and kinematics during the thaw season along a set of adjacent hillslopes across a 2 km² watershed located on the southern Seward Peninsula, AK. The team used collocated temperature and resistivity measurements with a supervised learning technique to map the spatial distribution of permafrost along the adjacent hillslopes. Further, researchers acquired time series of deformation and temperature data with a dense, low-cost sensor network providing depth-resolved measurements to depths up to 1.8 m at 59 locations. During a five-month monitoring period, displacements of a few millimeters to tens of centimeters were recorded. A detailed analysis of the data allowed the team to highlight the different factors controlling the movements (incline, slope, aspect, thaw layer thickness, soil moisture and permafrost conditions). This study provides a better understanding of the mechanisms controlling permafrost distribution, hillslope movement, and the possible impact on soil C distribution and landslide hazard. Further, this study offers a new window into belowground geomechanical processes that are inherently difficult to observe and can lead to large heterogeneity in C storage and release.

Improving the Parameterization of Arctic Stomatal Traits in a Land Surface Model Using Empirical Field Observations and Optimality Theory

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The Arctic ecosystem is experiencing unparalleled warming as the result of global climate change, resulting in significant impacts to vegetation and soils and leading to an overall “greening” of the Arctic through increased shrub cover and accelerated permafrost thaw. Earth system models are the primary tool to forecast the complex coupling between the surface and atmosphere, where the underlying land surface models (LSMs) provide the means to simulate the contributions of the terrestrial ecosystems to nutrient, carbon (C), water (H₂O), and energy cycles. Of the vegetation processes simulated within LSMs, stomatal conductance (*g_s*), the

exchange of carbon dioxide (CO₂) and H₂O through small pores on vegetation called stomata, is one of the most critical processes to represent correctly as it fundamentally governs the exchange of C and H₂O between the atmosphere and vegetative layer. Limitations imposed by stomata help set the upper limit on both H₂O loss via transpiration (*E*), and photosynthesis (*A*) through stomatal limitation on C diffusion into the leaf. As such, *g_s* is a strong determinant of gross primary productivity (GPP), with uncertainty in the model parameters related to stomatal conductance (the stomatal slope and stomatal intercept) contributing to some of the largest model uncertainties in current projections of C and H₂O cycling in LSMs. In this study, researchers collected full-range stomatal response curves on eight arctic plant species, across a range of environmental conditions, and used these data, along with an accompanying foliar biochemical analysis, to estimate five key foliar model parameters (stomatal slope, stomatal intercept, SLA₀, *F_{LNR}*, and CN_L) for the two default Arctic plant functional types (PFTs) used in the E3SM land model (ELM). By using these updated parameter values within ELM, researchers were able to assess the impact of revised parameters on modeled C cycling and evapotranspiration (ET). Further, using the newfound understanding of controls on Arctic plant stomatal conductance, along with widely held assumptions about stomatal optimality, researchers tested different assumptions for the way in which the soil moisture stress on *g_s* and ET are represented in ELM, such as having soil moisture stress increase leaf-level water use efficiency. The team also evaluated the patterns in GPP, ET and soil moisture against satellite retrievals under the different simulation scenarios. The findings highlight the importance of accurately representing stomatal response to biotic and abiotic factors when modeling Arctic ecosystems and the importance of parameterizations that are specific to Arctic PFTs.

Virtual

An Ecosystem Mapping and Modeling Unit Approach for Snow Scaling

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Scaling is a ubiquitous challenge in Earth system models (ESMs). Clustering methods applied in permafrost studies are applied here as a tool to upscale snow characteristics from watershed (~km scale) to regional scales (~10s of kms), in a construct the research team is referring to as

ecosystem mapping and modeling units (EMMUs). The resulting products can be used to evaluate coarse-scale ESM results, and to improve the ESM to reflect subgrid cell variability in snow characteristics.

In this work, researchers focus on two basins on the Seward Peninsula in Alaska, drawing on a combination of field-based and remotely sensed observations collected over winter and spring in 2021 and 2022. Estimates of snow cover and duration as well as snow insulation are derived for approximately 275 points across the basins using measurements obtained from iButton temperature sensors placed at ground surface as well as air temperatures collected at meteorological stations at each basin. Peak snow depth within the basins was measured manually at approximately 7000 points in late March 2022.

EMMUs are derived using a k-prototype clustering method, selected for its ability to handle mixed data types. Features included in the EMMU construct are derived from Light Detection and Ranging (LiDAR) data collected in summer 2022, satellite imagery, and from vegetation maps developed for the area. Several cluster variations were developed using different selections of input features and evaluated for their relationship to snow characteristics. Features considered include topographic characteristics of slope, elevation, aspect, and curvature; as well as vegetative characteristics of height and density, shrub presence or absence, and plant community type.

While traditionally ecosystem types focus on plant communities, the research team's initial results indicate a clustering approach that includes additional features is a stronger predictor of snow characteristics than vegetation type alone. Additionally, the predictive capabilities of EMMUs regarding snow characteristics (e.g., depth, duration, insulation) are compared with those of a machine-learning (random forest) model.

Leveraging the relationship between EMMUs and snow characteristics may represent a simpler alternative to more computationally intensive methods of scaling snow from watershed-to-regional scales and potentially assist with informing ELM subgrid variability.

Virtual

Controls on Carbon Release from Arctic Thermokarst Landscapes: Changing Redox Conditions Driven by Soil Saturation and Drainage

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Thawing Arctic permafrost causes land surface subsidence and formation of thermokarst drainage channels and lakes, altering biogeochemical redox cycles and soil organic carbon (SOC) decomposition. Soil saturation promotes anaerobic microbial activity and changes the balance of carbon (C) released as dissolved organic carbon (DOC), carbon dioxide (CO₂), and methane (CH₄). There is uncertainty about the degree to which soil saturation and subsequent redox transitions will impact Arctic fluxes and how to represent connections with hydrology and microbial SOC decomposition in ecosystem-scale models. Researchers evaluated if soil saturation and drainage—and associated changes in oxygen (O₂), iron cycling, and microbial communities—contributes to enhanced SOC decomposition. Two column experiments were conducted to simulate saturation and drainage in soils collected from an inundated thermokarst channel and the adjacent upland tundra near Council, Alaska. Over three months, continuous measurements of O₂ and volumetric water content were paired with discrete measurements of porewater pH, DOC, and iron. Column headspace was sampled for CO₂ and CH₄. Results show that during draining the upland column had 70% higher CO₂ fluxes than the thermokarst column, likely due to faster drainage and higher O₂ concentrations; intermittent CH₄ release was also observed for the thermokarst column. During saturation, ferrous total iron increased, and pH decreased for both columns. DOC increased (150 mg/L to over 500 mg/L) in the top portion of the upland column during saturation, which likely contributed to 50% higher CO₂ fluxes during the second drainage. The thermokarst column did not release as much DOC, possibly due to previous release of labile under saturated conditions. Soil extractions indicate downward transport of organic-bound iron in the upland column. Soils with high water content had higher relative abundances of

hydrogenotrophic and methyltrophic methanogens and higher ferrous iron supported putative iron and methane oxidizers. This study underscores the importance of redox cycling in Arctic SOC decomposition. Continued research targeting changes in Arctic soil redox gradients should be explored to inform model development for simulating future scenarios resulting from permafrost thaw.

Pan-Arctic Representativeness for Site Selection and Model Evaluation

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Characterizing the complex interactions among climate, landforms, permafrost, hydrology, biogeochemistry, vegetation, and snow is important to understanding how the Arctic will evolve under a rapidly changing climate. The NGEE-Arctic project is designed to advance such a predictive understanding and to deliver a process-rich ecosystem model suitable for modeling the evolution of Arctic ecosystems in a high-resolution Earth system model. *In situ* measurements and observational data are required to inform model development, and an optimal sampling strategy is needed to characterize vegetation and soil states and their responses to climate. Using a collection of pan-Arctic climatic, topographic, edaphic, and vegetation data, researchers applied a quantitative multivariate machine-learning methodology to stratify environmental gradients into ecoregions, which serve as potential sampling domains, and to determine the representativeness of eddy covariance measurement and soil and vegetation sampling sites. Data from tundra and boreal regions were included in the analyses, and about a dozen unique domains were identified across the eight countries encompassing Arctic tundra. Maps of ecoregions were produced, and the relative representativeness of available sampling sites in providing pan-Arctic coverage of carbon, water, and energy data was estimated. These analyses provide quantitative information about the spatial and temporal coverage provided by each sampling location and will be used to inform site selection for phase four of NGEE-Arctic. Moreover, the multivariate approach offers a quantitative method for up-scaling measurements, downscaling models, and identifying locations where additional measurements might greatly enhance model process representations.

Virtual

Potential of the Thermokarst Development at the Council Research Area

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As a climatically driven phenomenon, permafrost is undergoing degradation following global trends of air warming. Depending on the ground ice content, this might be realized in two ways: (1) formation of taliks (perennial unfrozen horizon between seasonally frozen layer and permafrost) when ice content does not exceed soil porosity and (2) formation of thermokarst, i.e., subsidence and collapsing of the ground surface due to melting of excessive ground ice. This case study estimated the potential for thermokarst development in the tundra at Council on the Seward Peninsula, Alaska. A deep, frozen core 6.7 meters long was collected in June 2017. The core was subsampled and analyzed for cryostratigraphy and basic soil properties such as total and dry bulk soil density and volumetric ice content.

A borehole was instrumented for long-term geothermal measurements. In June 2022 the team conducted a very low frequency geophysical survey combined with greenhouse gas flux measurements along a transect spanning an undisturbed peat plateau, a disturbed drilling site, and a natural thermokarst hollow. The core consists of the modern peat horizon about 70 cm thick, composing the active layer, and is underlain with mineral soil changing in texture from silt to sandy loam and then to sand and gravel. Volumetric ice content in this horizon of permafrost gradually decreased downward from ~70% to ~40%. Sustained increasing of permafrost temperature at a rate of about 0.05°C per year was recorded. This led to the formation of talik ~3 meters deep, which had been refrozen during the winter of 2019 to 2020 but thawed again in 2021 and kept developing. As a result, a local depression ~50 cm deep had formed. Vegetation had changed from tundra (moss, lichens, evergreen, and deciduous shrubs) to sedge wetland (cotton grass). Based on existing data about ice content, ground surface subsidence can be estimated at as much as 25% of the thaw depth increment. High methane flux recorded at the drilling site confirms that development of the thermokarst process converted the peat plateau from carbon sinking to greenhouse gas release. Methane production took place permanently within the 3-meter deep talik during entire year. Ongoing thermokarst processes can provide an excellent natural experiment that models consequences of further permafrost degradation in

terms of greenhouse gas release. Two sets of core subsamples are available for biogeochemical, microbiological, and hydrochemical analyses.

Remote Sensing–Based Mapping and Scaling of the Low Arctic Tundra Plant Functional Types and Classes from Field Plots to Peninsula

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High-resolution maps of vegetation distribution are crucial for studying the impacts of climate change on Arctic tundra ecosystems and their associated feedbacks. Bridging scales and integrating field-scale observations, airborne remote sensing and environmental datasets, researchers studied the current distribution and potential future changes in vegetation cover class and plant functional type covers across the low Arctic region of northwestern Alaska. Leveraging airborne hyperspectral imagery collected by NASA's Arctic-Boreal Vulnerability Experiment (ABOVE), the research team developed deep neural network-based models, trained using field vegetation surveys conducted at NGEE-Arctic intensive sites at Seward Peninsula, to develop a high resolution (5 m) landscape scale vegetation class maps with accuracy exceeding 93%. Analysis shows that the low- and mid-elevation areas on the landscape are dominated by shrubs and graminoid, while the high elevation areas are often dominated by dryas-lichen and nonvegetated classes. The team also developed random forest-based multivariate environmental niche models to determine habitat suitability of vegetation classes and further upscale the vegetation class mapping to regional scale across southern Seward Peninsula. Using future projections from five Earth system models (RCP8.5, CMIP5), researchers developed projections of vegetation cover classes in future decades up to 2050. Results show a substantial increase in shrub-dominated vegetation classes, especially along hillslope and high-resource environments like floodplains and stream corridors. Using plot observations of plant functional type cover, researchers have

developed model-ready data of fractional plant functional types at various resolutions to parameterize regional scale simulations of the ELM-Arctic model.

Predicting the Impact of Climate Change and Fire on Arctic Vegetation: FATES Modeling and Satellite Remote Sensing

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Climate warming and disturbance are expected to lead to large changes in the distribution of plant communities in the Arctic. Vegetation change is challenging to predict, as it is driven by the interplay of chronic climate trends, such as warming, disturbance by wildfire and thermokarst, and transient demographic processes of recruitment, growth, competition, and mortality. While most simulation models focus on the impacts of chronic climate trends, the roles of demographics and disturbance are poorly represented.

The research team seeks to improve the understanding and modeling of vegetation response to climate, subsurface conditions, and fire. To capture demographics and recovery from disturbance, researchers are developing the E3SM Land Model (ELM) coupled with the Functionally Assembled Terrestrial Ecosystem Simulator (ELM-FATES) for the Arctic. The team simulated vegetation demographic dynamics at the NGEE-Arctic Kougark Hillslope field site in Alaska under historical (1960 to 2010) and future (2051 to 2100) climates using ELM-FATES. Researchers identified a diverse set of trait combinations that all reproduce *in situ* observations of plant function type (PFT) composition under historical climate. However, under future climate, these trait combinations lead to drastically divergent compositions and productivity, resulting in trait-induced uncertainties that are three times larger than the effect of climate itself. The variation in PFT composition is primarily explained by traits controlling recruitment, growth strategy, and freeze-induced mortality. The findings highlight that accounting for demographic dynamics and additional observational constraints on key functional traits will contribute to constraining uncertainties in predicted vegetation change and carbon sink strength in northern-high latitudes.

Arctic wildfires, which are increasing in extent and severity, may be an important driver of vegetation shifts. Previous studies have used satellite imagery and machine learning to characterize Arctic land cover change, but not for post-fire recovery. Researchers studied the largest recorded tundra fire—the 2007 Anaktuvuk River Fire in northern Alaska—as a case study. The team used Landsat 7 imagery and a random forest model to generate annual maps of PFTs at 30 m resolution for 2007 to 2020. The model is constrained by ground surveys collected by the Bureau of Land Management. One year after the Anaktuvuk River Fire, shrub cover increased in burned areas but not in unburned areas. The maps in this poster are among the first quantifying decadal Arctic vegetation recovery trajectories at a high spatial resolution, which can be used in future work to identify greening trends, vegetation communities, and the expanding shrub line.

Changes in Seasonal Surface Energy Balance of High-Latitude Ecosystems Under Warmer Climate

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With rapid climate warming, expected changes in high-latitude vegetation and snow-pack dynamics may alter the surface albedo. The extent to which changes in surface albedo may alter surface energy balances and thus soil temperatures of northern ecosystems is uncertain. Researchers applied a processes-rich ecosystem model (EcoSys) to examine changes in seasonal surface energy balance driven by changes in albedo across Alaska. Under a warmer 21st century climate, surface albedo was modeled to decrease mainly during spring. This decline is particularly driven by increases in snow-free periods and extended length of growing season. Despite a decline in spring albedo, researchers modeled a slight increase in summer albedo as a result of vegetation change that led to a higher proportion of aspen, which was modeled to have a higher leaf albedo than black spruce in the boreal forest. Modeled latent heat fluxes were generally shown to increase, particularly during spring and summer. Overall, these changes in energy fluxes resulted in $3 \pm 0.34^\circ\text{C}$ increase in spatially averaged surface soil temperatures across Alaskan ecosystems by the year 2100.

Researchers conclude that seasonal changes in surface energy fluxes of northern ecosystems under warmer climates are primarily driven by vegetation and snowpack dynamics.

Virtual

Assessment of Changes in Permafrost and Ground Temperature in the Alaskan Arctic and Yamal Peninsula from 1900 to 2100

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Thawing and freezing of arctic soils is affected by many factors, with air temperature, vegetation, snow accumulation, and soil moisture among the most significant. Researchers employed the transient permafrost dynamics model developed at the Geophysical Institute Permafrost Laboratory (GIPL) and simulated several high spatial resolution (0.8 km × 0.8 km) scenarios of changes in permafrost characteristics in the Alaskan Arctic Brooks Range and Russia's Yamal Peninsula in response to projected climate change and land surface disturbances commonly occurring during various construction phases. Impacts of these changes in permafrost on northern ecosystems and infrastructure were assessed and regional maps of the possible impacts developed.

The GIPL-2 model numerically simulates soil temperature dynamics and the depth of seasonal freezing and thawing by solving the one-dimensional, non-linear heat equation with phase change. In this model, the processes of soil freezing and thawing occur in accordance with the volumetric unfrozen water content curve and soil thermal properties. Snow temperature and thickness dynamics were simulated assuming snow accumulation, compaction, and phase change processes. Model simulations were validated by comparison with available active layer, permafrost temperature, and snow depth records from existing permafrost observatories operated by the U.S. Geological Survey and the Geophysical Institute. Properties of surface vegetation, soil type, layering, and moisture content were up-scaled using Sentinel-1 and Sentinel-2 satellite maps of Ecosystems of Northern Alaska, Arctic Network of Parks and Preserves, and Land Cover Classification.

Spatially Resolved Projections of Permafrost Thaw, Microtopography Change, and Landscape Hydrology for a Polygonal Tundra Site

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Microtopography change caused by melting ground ice has been identified as a mechanism that could accelerate permafrost thaw in polygonal tundra. Researchers used the integrated surface and subsurface cryohydrology Advanced Terrestrial Simulator (ATS) to investigate the effect of that positive feedback mechanism. ATS solves coupled equations for surface and subsurface thermal hydrology and includes representations of subsidence caused by melting excess ice and resulting effects on microtopography. The simulations of a polygonal tundra site near Utqiagvik, AK were informed by spatially averaged depth profiles of permafrost ice content, an important control on the rate of subsidence, which were estimated from intensive sampling of transects across six ice-wedge polygons (from trough center to trough center). The simulations build on previous small-scale ATS simulations that agree well with multiyear observations of snow depth, suprapermafrost water table depth, and depth-resolved soil temperature. The new simulations of a small catchment comprising 468 ice wedge polygons agree well with published estimates of landscape runoff, evapotranspiration, and subsidence. Projections indicate 63 cm of bulk subsidence from 2006 to 2100 in the RCP8.5 climate. Permafrost thaw, as measured by the increase in active layer thickness, is not accelerated significantly by subsidence. Projected active layer thickness at year 2100 is approximately 180 cm when subsidence is included compared to about 160 cm when it is neglected. However, if thaw is measured by the amount of previously frozen carbon that thaws each summer, subsidence has a greater impact; the amount of soil solids thawing each summer is roughly 65% higher in the subsiding case compared to the nonsubsiding case. In these simulations, previously identified positive feedbacks between subsidence and thaw are self-limiting on decadal time frames because microtopographic change caused by melting ground ice, specifically, the transitions from low-centered to high-centered polygons, decreases depression storage and increases landscape runoff, resulting in

drier tundra with weaker surface and atmosphere coupling. Those changes in hydrology help maintain stream flows in a warming climate but also lead to drier tundra conditions.

Painter, S.L., et al. 2023. "Drying of Tundra Landscapes will Limit Subsidence-Induced Acceleration of Permafrost Thaw," *Proceedings of the National Academy of Sciences* **120**, e2212171120.

Warming and Thawing Permafrost in Alaska

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The impact of climate warming on permafrost and the potential of climate feedbacks resulting from permafrost thawing have recently received a remarkable attention. Climate warming promotes an increase in permafrost temperature and active layer thickness, which in turn affect the stability of northern ecosystems, threaten infrastructure, and cause the release of carbon dioxide and methane into the atmosphere. The timing and rate of permafrost degradation are two of the major factors in determining the anticipated negative impacts of climate warming on the Arctic ecosystems and infrastructure. This project presents the results of almost 40 years of permafrost and active layer temperature observations in Alaska. Most of the sites in Alaska show substantial warming of permafrost since the 1980s. The magnitude of warming has varied with location, but was typically from 0.5 to 4°C. However, this warming was not linear in time and not spatially uniform. While permafrost warming was more or less continuous on the north slope of Alaska with a rate between 0.2 to 1°C per decade, permafrost temperatures in the Alaskan interior started to experience a slight cooling in the 2000s that has continued during the first half of the 2010s. The warming resumed in the mid-2010s. By 2020, new record highs for the entire period of temperature measurements at 15 m and 20 m depth were recorded at all locations. This warming has triggered near-surface permafrost degradation and talik development in many locations in the Alaskan interior and in the northwest of Alaska with adverse consequences for ground surface stability. The talik starts to form when the depth of potential seasonal ground thawing exceeds the depth of potential freezing. To enhance the understanding of possible future rates and pathways of permafrost degradation and to predict the local, regional, and global consequences to human society, accurate high spatial resolution permafrost models are needed. Establishment of these models is possible only by integrating available high-resolution

environmental data and by assimilation of existing field and remote sensing data and observations into these models. A Geophysical Institute Permafrost Laboratory (GIPL2) model, a high-resolution stand-alone permafrost dynamics model, will be used to illustrate how changes in climate together with further industrial development of the north slope of Alaska will affect permafrost and ecosystems in this region.

Coupled Landscape and Ecosystem Response to Permafrost Loss and Disturbance

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The rapid and catastrophic erosion of soil on hillslopes underlain by permafrost has been attributed to rapid deepening of seasonally thawed surface material and the loss of near-surface permafrost. These erosional events both redistribute sediment, reshape hillslopes, and have the potential to abruptly release globally significant quantities of soil carbon (C) from previously stable sinks. At a series of small watersheds on the southern Seward Peninsula in Alaska, researchers have documented a range of soil movement processes affected by the presence and recent loss of permafrost. These movements range from steady creep-like behavior to rapid and repetitive failures. Based on direct field measurements and geophysical imaging of the sub-surface conducted over multi-year campaigns, researchers produced high-resolution maps showing the presence and absence of near-surface permafrost across these watersheds. A comparison of the permafrost map to the spatial patterns of annual ground surface displacement and failures suggests that regions of recent and/or active permafrost loss exhibit the greatest rates of movement measured from 2017 to 2022. Despite topographic evidence of past failures, regions without permafrost have the lowest rates of present-day movement. Regions of relatively stable and continuous permafrost have intermediate rates of soil creep and lack catastrophic erosional features.

The loss of permafrost drives both an increase the heterogeneity in microtopography and the diversity and spatial complexity of vegetation. Topographic heterogeneity arises from local ground subsidence, Earth flows, and retrogressive failures propagating across recently thawed hillslopes with topographic connectivity to rapidly eroding stream hollows.

Vegetation heterogeneity associated with disturbance is evidenced by shrubification of stream hollows experiencing active gullying, on the margins of solifluction and Earth flow lobes, and in active layer detachment scars. Despite steep hillslopes, Earth flow scars create areas of relatively flat topography that route and capture surface water runoff, leading to emergent patches of graminoids *Eriophorum vaginatum*, *Carex aquatilis*, and *Equisetum hyemale*.

Overall, the team's observations suggest that the greatest hillslope instability occurs in the transitional regions of watersheds undergoing rapid permafrost loss. Both the rates and extent of propagation of failures appears to be influenced by the topographic connectivity of failures to the network of established channels and developing gullies. If the small watersheds are representative of larger swathes of permafrost landscapes, then researchers expect to see an acceleration of hillslope processes and release of soil organic C during and immediately following permafrost loss followed by a reduction in soil transport rates and a stabilization of the landscape.

Wildfire Influence Impacts on Carbon Storage in Arctic Tundra

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Understanding the impacts of novel wildfire regimes on soil carbon (C) storage and fluxes is critical to improve the ability to predict the vulnerability of Arctic systems to disturbances. Increased wildfire activities reported in the Arctic can disrupt vegetation-soil dynamics and accelerate carbon dioxide (CO₂) emissions to the atmosphere, thereby increasing the vulnerability of permafrost C. Repeated burns and time since last fire are important when considering the response trajectory of ecosystems, especially when and under what conditions soils are a net C source or sink. The objective of this research is to measure the effects of fire frequency and time since last fire on soil C stocks and CO₂ efflux rates from an Arctic tussock tundra ecosystem. Researchers hypothesize that stocks and fluxes will be more affected by repeated burning than by time since last burning, with more frequent burning leading to decreased total C stocks but increased fire-derived (pyrogenic) C stocks. Pyrogenic C is more stable in soil compared to bulk soil C and is considered an important carbon sink. The team also hypothesize that an increase in fire frequency will decrease CO₂ flux rates from soils. In 2022, researchers measured

organic layer thickness and thaw depth, and sampled organic layers from the Kougarok fire complex near Nome, AK from unburned sites and sites burned at different years (1971 and 2002) and more than once (twice: 2002 and 2019; three times: 1971, 2002, and 2019; and four times: 1971, 1997, 2002, and 2015). Organic layer samples were dried, ground, and will be analyzed for total elemental C and pyrogenic C. Researchers will present results for C stocks across the different fire treatments at Kougarok fire complex and the plan for soil CO₂ efflux measurements at those sites in summer 2023.

Simulating Arctic Vegetation Distributions and Biogeochemical Processes in the E3SM Land Model

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A major goal of the NGEE-Arctic project is to integrate improved scientific understanding of Arctic systems into the Energy Exascale Earth System Model (E3SM) to connect scientific discoveries from observations, experiments, and detailed modeling of the Arctic into global-scale predictive models. New understanding of Arctic processes is being incorporated into hydrological, physical, biogeochemical, and vegetation process modules in the E3SM Land Model (ELM) through multiple integrative modeling efforts as part of NGEE-Arctic phase three.

Researchers have conducted spatially explicit simulations of vegetation distributions across three intensively studied field sites in the Seward Peninsula, AK. Recent ELM updates incorporated nine tundra-specific plant functional types (PFTs), several of which are new to the model, including nonvascular mosses and lichens, graminoids, forbs, and shrubs of various height classes as well as a nitrogen-fixing alder shrub. The spatially explicit vegetation simulations combine parameterization based on extensive field sampling of vegetation biomass and traits with remote sensing-based mapping of vegetation distributions to drive model

projections of how vegetation carbon (C) stocks, net primary production, and nutrient cycling vary across space and time in areas with contrasting climate, topography, and soil properties.

Researchers have implemented new soil biogeochemical capabilities into ELM with the goal of better representing greenhouse gas production across complex tundra landscapes. The team has used a new, direct coupling between ELM and the reactive transport simulator PFLOTRAN to integrate a reaction network combining soil organic matter decomposition with pH dynamics, iron redox cycling, oxygen consumption, fermentation, and methanogenesis into ELM soil columns. The team then simulated coupled C, oxygen, and iron redox cycling in polygonal tundra soils at the Barrow Environmental Observatory in Utqiagvik, AK and evaluated simulations using measured profiles of pH, C, nitrate, iron, and sulfate as well as surface methane (CH₄) and carbon dioxide (CO₂) fluxes from nearby polygonal tundra sites. Directly integrating subsurface geochemical interactions into ELM allows process-based simulation of variations in CO₂ and CH₄ production across gradients of redox state, terminal electron acceptor availability, and soil geochemical properties. Altogether, these developments translate discovery science from a range of above- and belowground observations, experiments, and detailed modeling studies within the NGEE-Arctic Project into concrete improvements in E3SM modeling capabilities.

Metagenomic Insights into Decadal Changes in Carbon and Nitrogen Cycling in Arctic Tundra Biomes

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This project uses state of the art sequencing and imaging technologies to resolve complex interactions governing the biochemical cycles in tundra biomes to better inform efforts to decipher arctic carbon (C) and nitrogen cycling. Arctic soils are among the largest terrestrial C stores in the world, making them a critical focus for climate change research. However, rising global temperatures could cause rapid microbial mineralization and increased greenhouse gas (GHG) emissions from these C stores. Various landscape

features, including soil surface and subsurface slope, redox gradients, ice wedge formation, and permafrost depth, create diverse microbial habitats that may respond differently to warming and perturbations. The seasonal changes in soil microbiomes and their impact on GHG production potential remain poorly understood.

Between 2011 and 2022, researchers conducted multiple sampling campaigns to collect active layer soils from the polygonal arctic tundra at the Barrow Environmental Observatory (BEO). The team analyzed the chemical and biological properties of these soils and monitored greenhouse gas (GHG) emissions. To better understand the microbial communities in these soils, researchers extracted and sequenced the whole community DNA, resulting in several hundred metagenome-assembled genomes (MAGs) and viral genomes (vMAGs). In addition, the team analyzed the soil biochemistry to better understand the relationship between soil properties and microbial communities via synchrotron fourier transform infrared (SR-FTIR) spectral imaging at the Berkeley Infrared Structural Biology beamline of the Advanced Light Source (LBNL).

At the study location, the microbiomes of the tundra are organized according to topographical features, which has a direct impact on the distribution of key genes responsible for greenhouse gas (GHG) emissions. Researchers found that the potential for GHG production was localized and varied greatly between different polygons. The analysis of microbial genomes revealed that they have an improved resilience to changes in C availability, fluctuating temperatures, and nutrient-deficient conditions in tundra soils. While microbial communities did exhibit seasonal variations, landscape topography remained the main factor distinguishing the distribution of microbial functions over a thaw season. Integrating microbial functions with geochemistry and GHG fluxes enhances the understanding of how landscape topography shapes biogeochemical cycles in Arctic soils. This approach can help better predict the ecosystem responses to climate change and reduce uncertainties in future projections.

Virtual

High-Resolution Maps of Near-Surface Permafrost on the Seward Peninsula, Alaska, Generated with Machine Learning

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<https://ngee-arctic.ornl.gov/>

Permafrost soils are a critical component of arctic ecosystems and the global carbon cycle, as they store vast amounts of carbon. They are also important on a regional and local scale, in part because they regulate water flow from uplands to rivers and oceans. Hence, identifying the distribution of permafrost soils is crucial to understanding local- to global-scale impacts of permafrost thaw. Regional and hemispherical maps of permafrost distributions are typically generated at the scale of tens of meters or kilometers. This is too coarse to resolve permafrost distributions to a scale needed to identify processes driving degradation, to assess infrastructure stability, or to illuminate geomorphic impacts of permafrost thaw such as soil carbon transport dynamics. Here, the team developed a machine-learning (ML) model to generate meter-scale maps of near-surface permafrost distributions for the watersheds within the discontinuous permafrost region of the Seward Peninsula, AK. Ground-truth observations of the near-surface permafrost extent were determined in three watersheds using measurements of soil temperature from 0.75 to 1.2 m depth, electrical resistivity tomography, and observations from soil pits and frost probing. To predict the full distribution of near-surface permafrost at each of the three watersheds, a ML model was trained using the ground-truth observations, topographic and vegetation metrics derived from lidar point clouds, and multispectral indices for snow cover derived from high-resolution satellite imagery. Specifically, two ML models were trained: extremely randomized trees (ERTr) and a support vector machine (SVM). The transferabilities of the trained ML models were tested by running the models at sites where the models were not trained. Near-surface permafrost distributions predicted by the ERTTr produced the highest balanced accuracy (BA) at the training site ("at-a-site") (BA>90%). However, the transferability of the ERTTr to other sites was low, with BA ranging from 50 to 60%. The SVM had lower accuracies for at-a-site prediction (BA=70 to 80%), yet greater accuracy when transferred

to the non-training site (BA=70 to 80%). The accuracy of these models demonstrates that integrating geophysical measurements with topographic and multispectral data into a ML model provides a promising approach to generating fine-scale maps of permafrost distributions where sufficient ground-truth data exist. However, producing high-resolution permafrost extent maps across larger spatial scales remains challenging because of site specific variability in drivers of permafrost degradation.

Scaling Knowledge of Arctic Tundra Processes from Field Studies and Fine-Scale Models to an Earth System Model

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The overarching objective for the 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) gridcell. To achieve that goal, researchers have identified six Integrated Modeling (IM) efforts, each of which results in improved prediction capability implemented within the DOE's Energy Exascale Earth System Model (E3SM). During phase three of NGEE-Arctic, researchers are synthesizing observations, experimentation, and fine-scale modeling results to arrive at new ELM parameterizations suitable for a high-resolution ESM gridcell. The product of each IM effort is an updated code module that extends the default capability of the E3SM Land Model (ELM). Researchers are currently targeting a 1 km × 1 km ELM gridcell size for this work, which is the most highly resolved land grid that is currently planned for continental-to-global scale simulations with E3SM. The six IM efforts focus on improved representations of the following important drivers of energy-water-carbon-biogeochemistry interactions in tundra landscapes: (1) fractional inundated area; (2) hillslope processes; (3) snow-terrain-vegetation interactions; (4) tundra-specific plant functional types;

(5) dynamic biogeography; and (6) biogeochemistry in variably saturated soils. Researchers are making extensive use of the existing multilevel hierarchical subgrid capability of ELM to capture new knowledge about variability at scales finer than the 1 km grid, and the team is putting in place strategic extensions of that subgrid capability as needed to represent Arctic tundra ecosystems. The results for each IM effort are shown, demonstrating how observations, experimentation, and fine-scale modeling are producing improved performance within ELM compared to a baseline implementation without Arctic-relevant parameterizations.

NGEE-Arctic Project Transfer of Datasets, Model Products, and Digital Object Identifier Ownership Developed in Phase 1–3 to the ESS-DIVE Long-Term Repository

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NGEE-Arctic will finish the third phase of the project at the end of FY24 with a deliverable of transferring all the NGEE-Arctic project archive datasets to the ESS-DIVE repository for long-term archive and management of Earth and environmental science data. In October 2022, the Data Management Team (DMT) presented a close out timeline to the project team based on quarterly accomplishments with the goal of publishing all current, public NGEE-Arctic data packages and model products to ESS-DIVE by the end of calendar year 2023. There is a concurrent effort to finalize and release to the public any dataset or model product that is currently shared with the team only. For future time and effort planning purposes, the DMT developed a backlog inventory spreadsheet being populated by the researchers to identify datasets in preparation for submission.

The DMT and Data Representatives at each institution will increase efforts to assist researchers in organizing, finalizing, and documenting packages for ingest and public release under the CC-BY 4.0 license. Ingest and transfer efforts are tracked on the collaborative work management tool, Trello. Early project archived data packages and model products will be reviewed and updated to meet the metadata requirements at ESS-DIVE. The more recent submissions will have the minimum reporting formats applied for CSV Structure and File-level Metadata and, as appropriate, Model Data and UAS.

The DMT plans for a transition to ingesting data packages and model products directly with ESS-DIVE prior to the close out while continuing to assist project researchers in the ingest process and maintaining the project archive of the metadata and data. This change in submission workflow will need to be well thought-out and shared with the project team.

Data will be available in the ESS-DIVE data portal and the customized NGEE-Arctic archive data portal on the ESS-DIVE site and the NGEE-Arctic website. Throughout the close out, the DMT will be working collaboratively and seeking guidance from ESS-DIVE staff in resolving technical issues, transfer and publishing workflows, and in updating packages to meet repository guidelines and requirements. The DMT and ESS-DIVE are also working closely with Office of Scientific and Technical Information (OSTI) staff on the process of transferring the “releasing official” role from NGEE-Arctic to ESS-DIVE for Digital Object Identifiers (DOIs) and updating the DOI records to reflect necessary changes.

Characterizing Fine-Scale Landscape Controls on Patterns of Arctic Plant Phenology Using High-Resolution Remote Sensing

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The timing of seasonal plant leaf growth, expansion, and senescence—known as leaf phenology—is highly sensitive to environmental conditions and is a strong control of annual fluxes of carbon, water, and energy. In the high-latitude Arctic, the air is warming two times faster than the rest of the planet, driving changes in both the onset and duration of plant phenological events (e.g., earlier leaf-on and delayed leaf-off). However, differences in observed phenological timing across warming experiments, long-term ecological research, and satellite records due to differences in scales, approaches, and collection periods have strained the ability to understand the primary drivers of plant phenological response to climate and to correctly represent them in process models. Researchers hypothesize that a major reason for the mismatch between observations is the neglect of the significant landscape-scale spatial variability

in phenology driven by fine-scale landscape characteristics (e.g., vegetation composition, snow seasonality, topography, permafrost, and soil moisture). Improved understanding of these fine-scale interconnections between plant phenology and landscape characteristics is important but remains limited due to challenges associated with deploying *in situ* observational equipment or the use of coarse resolution (spatially and temporally) time-series satellite observations.

To address this challenge, researchers deployed 26 custom phenocam systems (PiCAM) that were designed for long-term unattended operations at three low-Arctic tundra sites on the Seward Peninsula, Alaska. Combining data from these PiCAMs and high-resolution (3 m) PlanetScope CubeSats, researchers investigated phenological variations across 12 Arctic plant functional types (PFTs) and their associations with landscape characteristics. The team found that both spring and fall phenology differed strongly across PFTs (by up to 20 days in leaf-on and 40 days in leaf-fall). In particular, deciduous tall shrub species (alder and willow) displayed a later spring green-up (~7 days behind the mean of other PFTs) but completed leaf expansion much faster than other PFTs (within only ~10 days). In contrast, dry tussock graminoids had an earlier start of spring green-up but maintained slow progressive growth during the season. Researchers found that the variation in spring phenology across space and time was strongly coupled with the timing of snowmelt, as well as topography and geomorphological features that affected vegetation and soil moisture distribution. The findings highlight a critical need to characterize Arctic plant phenology at the landscape scale to gain an improved understanding of the fine-scale controls on phenology and species distribution to better represent these processes in ecosystem process models.

Data and Model Integration for High-Resolution E3SM Land Model in Northern High-Latitude Regions: A Demonstration at the NGEE-Arctic Seward Peninsula Sites

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In the high-latitude Arctic, modeling land surface processes (e.g., snow process, phenology, and consequent soil and plant responses) is a great challenge in the Earth system, mostly due to a highly heterogeneous surface across scales and the lack of consistent, reliable data in both space and time series. In this study, researchers present an integrative data and model workflow to synchronize inputs and driving forcings from varied sources for offline high-resolution (1 km×1 km or finer) land surface simulations using the Energy Exascale Earth System Model (E3SM)'s Land Model (ELM).

As an example, this workflow is applied over the Seward Peninsula, AK, covering NGEE-Arctic Intensive Sites, at either 100 m × 100 m or 1 km × 1 km spatial resolution. Offline ELM is driven by GSWP3 (Global Soil Wetness Project Phase 3) v2 forcing data spatially downscaled to 1 km×1 km with Daymet v4 from 1980 to 2014 (<https://daymet.ornl.gov/>). High-resolution surface properties include: (1) topography (elevation, slope, aspect) at a 5 m × 5 m resolution (<https://www.pgc.umn.edu/data/arc-ticdem/>); (2) 3 min × 3 min soil thickness (https://daac.ornl.gov/SOILS/guides/Global_Soil_Regolith_Sediment.html); (3) 3 min × 3 min lake and glacier fractions; and (4) 250 m × 250 m soil clay, sand, and organic matter content from SoilGrids (<https://soilgrids.org>). Furthermore, a newly developed arctic plant function type (PFT) dataset, derived from field investigations and remote sensing, is incorporated as well. This PFT data product is tightly associated with model development and its parameterization in targeted terrestrial ecosystems (Sulman et al. 2021).

The integrated data and ELM are in testing and evaluating, and preliminary results show reasonable simulations in the case study sites. After further and careful assessment,

workflow would be useful in ELM application for pan-Arctic region or others.

Sulman, B. N., et al. 2021. "Integrating Arctic Plant Functional Types in a Land Surface Model Using Above- and Belowground Field Observations," *Journal of Advances in Modeling Earth Systems*, 13(4), e2020MS002396. DOI:10.1029/2020MS002396.

Tree Damage as an Ecological Process: Evidence from a Pantropical Monitoring Program

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<https://ngee-tropics.lbl.gov/>

Forests are key to mitigating climate change. However, large uncertainties remain on how these ecosystems will respond to future environmental changes, especially in the tropics, where high species diversity implies different responses to a particular stressor. Here, evidence is presented of a key, but underappreciated, ecological process in the dynamics of tropical forests: tree damage. Observations were used from 29 annual mortality and damage censuses across seven tropical forest plots of the Forest Global Earth Observatory network in the neotropics and Asia to study the role that damage to living trees has on forest dynamics. Tree damage was one of the most important mortality risk factors and contributed to a substantial, yet rarely quantified, proportion of total forest biomass losses in these forests. Researchers also showed that conventional forest

inventories that ignore tree damage result in: (1) overestimates of aboveground biomass (AGB) stocks by 4% (1% to 17% range across forests) because they assume that trees are structurally complete, (2) underestimates of total AGB loss by 29% (6% to 57% range across forests) due to overlooked damage-related AGB losses, and (3) overestimates of AGB loss via mortality by 22% (7% to 80% range across forests) because of the assumption that trees are undamaged before dying. Damage on living trees is likely to become more important as the frequency and severity of forest disturbances increase.

Data Synthesis and Management Activities for NGEE-Tropics

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<https://ngt-data.lbl.gov/>

The two main data-related activities of NGEE-Tropics are providing data archiving for project data via the NGEE-Tropics Archive and performing data curation and synthesis. This presentation highlights recent data archive developments including streamlining dataset creation workflows, which facilitates usage by data contributors by automating much of the work. For instance, digital object identifiers (DOIs) are now automatically created, becoming immediately available to data contributors once the dataset is submitted for review. The project also reviewed best practices aligned with community established formats, allowing for any potential issues, like incomplete information for metadata fields, to be caught early in the dataset publication process. The research team showed usage metrics for datasets deposited, number of system users, data downloads, and size and variety of data deposited. The large variety in the types of data deposited enabled team involvement in the creation of new data and metadata formats and standards, particularly in collaboration with other ESS-funded projects like ESS-DIVE and AmeriFlux. Other new features have also helped improve the overall process, such as versioning for datasets and enabling easy updates and corrections, and support for draft datasets, raw data, and partner data, which might have accessibility restrictions. All these improvements are aimed at making data archiving an integral part of the regular scientific workflow for the project. From the long-term data preservation perspective, the NGEE-Tropics Archive is now fully integrated with ESS-DIVE, the official

long-term repository for ESS data. All public-access datasets are now synchronized with ESS-DIVE, and new datasets are synchronized in near-real-time with publication in the NGEE-Tropics Archive. With that, long-term preservation of NGEE-Tropics data is ensured, while still fully supporting team needs. Data curation activities included synthesizing and quality controlling several datasets used in recent publications for the project, including sap flow, micrometeorology, soil measurements, leaf-level measurements, and others. For instance, forest inventory data from BIONTE, a 30-plus-year logging experiment in Manaus, underwent quality control, integration of data from multiple sources, and georeferencing of every tree, enabling the team to better prepare for field campaigns.

The Role of Soil Nutrient Status in Regulating Biomass Fluxes in Lowland Tropical Forests

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The role of soil nutrient status in regulating the dynamics of tropical forests remains poorly understood. Accurate predictions of tropical forest structure and responses to changing climate, rising carbon dioxide, and disturbance require a much deeper understanding of the interplay between soil nutrient availability and forest production, function, and functional composition. In addition to soil nutrients, tree size is another driver that shapes forest carbon dynamics and determines the interaction between trees and the environment. Small trees have larger contributions to biomass fluxes, i.e., woody productivity (AWP) and woody mortality (AWM), compared to large trees, which dominate biomass stocks. This preliminary study used long-term Barro Colorado Island (BCI) data coupled with a detailed soil survey, including measurements of phosphorus (P), aluminum, iron, magnesium, and manganese (Mn) concentrations, to assess whether soil nutrient availability regulates biomass fluxes as a function of tree size. AWP varied among size classes, being lower at larger size classes, and had a negative association with Mn, suggesting that a high solubility and uptake of toxic metals (e.g., Mn) by trees may constrain productivity. No association of AWP with P was observed, which is expected to limit productivity in tropical forests. This lack of association between P and AWP is consistent with experiments and observations in areas near BCI where it has been suggested that a lack of community-level variation in productivity in relation to P may result from strong species turnover. Moreover, AWM was not related

to variation in soil fertility but differed among size classes. However, differences in AWM among size classes were random, suggesting a strong role of stochastic processes in AWM. This analysis will be replicated at the pantropical level by including sites with a larger variability in soil nutrient availability from the Forest Global Earth Observatory network. This work will enable the evaluation and benchmarking of Earth system model nutrient cycle representations by providing pantropical empirical representations of the role of soil nutrient status in regulating the dynamics of tropical forests.

No Variation of Leaf-Level Water Use Efficiency Along the Fast-Slow Growth Spectrum in Amazonian Forest Trees

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Forest disturbance increases the proportion of fast-growing species compared to slow-growing species. These two species groups have different carbon storage capacities and different vulnerabilities to climate change. Understanding physiological differences between these groups is necessary to enabling their representation as separate plant functional types within Earth system models. This study analyzed leaf-level water-use efficiency—the marginal carbon gain of transpiration water loss which controls leaf gas exchange. Wood density was used as a proxy for the fast-slow growth spectrum to test whether low wood density trees (LWD) had a lower leaf water-use efficiency than trees with a high wood density (HWD). At one Amazonian forest site, *in situ* steady-state gas exchange measurements and leaf composition measurements were performed on sun-lit leaves of five LWD and five HWD species. LWD species invested more nitrogen in photosynthetic capacity than HWD species and had higher photosynthetic rates and higher stomatal conductance. However, the two groups had a comparable leaf water-use efficiency. This has implications for the physiology of tropical trees and for developing separate fast-growing and slow-growing plant functional types in

Earth system models. The study also showed that waiting for steady-state gas-exchange markedly increased estimates of leaf water-use efficiency.

A New ESS-DIVE Reporting Format for Unoccupied Aerial Systems Data and Metadata

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The use of small unoccupied aerial systems (UASs) as an aerial platform to collect novel high-resolution data and address a wide range of tropical research questions is a rapidly developing field. Applications in tropical ecosystems include the collection of fine-scale information on tree species distribution, canopy structure, vegetation phenology, and disturbance dynamics to inform remote sensing and modeling studies. However, the lack of common metadata and formats that facilitate data interoperability is a major limitation to these efforts, making synthesis extremely challenging to achieve. ESS-DIVE is addressing these challenges by creating data and metadata reporting formats for domain-specific data types through its Community Funds program. The aim of this work is to develop open, standardized formats, vocabulary, and metadata requirements for the archiving of data from small UASs (≤ 25 kg). This includes basic recording of core flight data (e.g., telemetry) and primary flight metadata (e.g., flight paths, altitude, date, and time), UAS payload and instrumentation information (e.g., sensor types and specifications), and the data product metadata needed for interpreting and accessing derived UAS datasets (e.g., resolution and spatial reference system). The reporting format documentation includes a description of each proposed metadata element, with a variable name, unit, description, and example. To accommodate the diversity of platform types, instrumentation, and data collected, these elements are presented as a framework for users to adapt to their own needs rather than a rigid set of requirements. To better facilitate data discovery, categories of data products are proposed based on the level of data processing.

Each data level is described with examples and applicable file types. Data level classification will streamline identification of compatible products for data synthesis and improve data search effectiveness on the ESS-DIVE portal. Format documentation is open source and available at <https://github.com/ess-dive-community/essdive-uas>. All UAS

data generators and users are encouraged to provide input and make use of these resources. Draft documentation is currently available for feedback, and the project will be completed by September 2023.

Reaching the Holy Grail During the Tropical Wet Season: Accelerated Daytime Stem Growth and Respiration of Canopy Trees in the Amazon Basin

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Understanding how diurnal respiratory and growth rates of tropical trees respond to temperature in the dry and wet seasons is critical for accurately simulating the future of tropical forest dynamics. While methods to study growth and respiratory processes over diurnal time scales are lacking, this study hypothesized that tree growth rates and their associated respiratory loss rates of carbon dioxide (CO₂) are much more sensitive to mild tissue water-stress associated with transpiration than photosynthetic carbon assimilation processes in leaves. The study further hypothesized that stem wood growth and respiration, which accounts for the majority of tree biomass and a large fraction of autotrophic respiration, occurs mainly at night during the dry season and is associated with reduced transpiration rates and refilling of stem water storage capacity. During the day, high transpiration rates and reduced stem water potential result in insufficient daytime turgor pressure required for cell wall expansion and growth. This predicts a negative relationship between stem respiration and temperature. This also predicts that during the wet season, when transpiration is suppressed due to low vapor pressure deficits, increased daytime turgor pressure allows growth and respiration to accelerate as a function of temperature with a positive relationship predicted between stem respiration and temperature. These hypotheses were evaluated by developing a portable system for quantifying real-time stem CO₂ efflux rates (ES). Diurnal patterns were summarized in sap flow and ES during the dry and wet seasons in the central Amazon across fast- and slow-growing tree species. While previous work revealed an Amazon “green-up” during the dry season due to leaf flushing, this

study suggests that the holy grail for plants is achieved during the wet season, when temperature-stimulated photosynthesis and growth can occur in parallel during the day due to sufficient turgor pressure.

Climate Warming Leads to Increased Forest Burn Area and Deep Forest Penetration in the Amazon

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Amazonian fires have become more frequent and widespread under climate change, exerting a profound impact on society and ecosystems. In addition, edge effect promotes canopy loss and facilitates anthropogenic fires to escape into the forests, intensifying carbon losses. However, it is unclear how increases in extreme climate and forest edge area affects fire occurrence and spread. This study investigated the influence of land surface temperature (LST) on burn areas of evergreen forest across the Amazon basin from 2000 to 2020. The burn area of evergreen forest increased exponentially with the increase in LST from July to October. The forest edge was warmer and often had more burn areas than forest far from the edge (>8 km). Higher LST (>36 °C) is strongly correlated with more burn areas and deeper forest penetration distance from the edge. These findings indicate forest degradation leads to higher vulnerability at forest edges under a warmer and drier climate in the Amazon.

The Drivers of Coexistence and Dominance of Plant Functional Types Across the Neotropics: An Integrated Approach Using Model and Regional-Scale Trait Data

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Climate change is expected to increase the frequency of hot drought events across the wet and dry tropics. To understand how recurrent droughts impact tropical ecosystems, terrestrial biosphere models must represent the observed trait trade-offs between drought resistance and productivity. To investigate the mechanisms that determine the distribution of deciduousness (a drought avoidance strategy) and evergreenness across the neotropics, researchers implemented a drought-deciduous representation into FATES. To define regional-scale plant functional types (PFTs), researchers used over 20 traits from >4,000 tree species in the neotropics. An unsupervised cluster algorithm was used to define PFTs based on these traits, resulting in PFTs that differed by either deciduousness or successional stage. The team selected multiple sites across a mean annual precipitation gradient in tropical South America (500 to 3,000 mm/yr) to test whether the model could represent different levels of coexistence. The model successfully predicted the biomass distribution across sites, the higher abundance of tall trees in wet sites, and the higher abundance of drought deciduous trees at dry forest sites. FATES correctly represented the seasonality of evapotranspiration and gross primary productivity, except for the early dry season in dry forest sites. In contrast, the model overestimated the abundance of pioneer evergreen trees and could not represent

successional coexistence at moist tropical forests, suggesting that current parameterized trade-offs in moist forests are insufficient for representing coexistence. The study shows that incorporating existing trait observations can improve understanding of deciduous–evergreen coexistence across the tropics. However, more data and model processes are likely needed to better understand coexistence of multiple PFTs across successional gradients in moist tropical forests.

Root Nutrient Uptake Kinetics in Trees

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Global vegetation models increasingly represent the nutrient costs of plant growth. The parameters governing plant nutrient acquisition are therefore central to accurate carbon cycle projections, yet understanding of nutrient uptake has been limited by the difficulty of measuring root physiological traits. Root nutrient uptake is often described by two Michaelis-Menten parameters: maximum uptake rate (V_{\max}) and substrate affinity (K_m). These parameters may vary by plant functional type or with environmental conditions. Plants may alter nutrient uptake kinetics in response to nutrient limitation or, over longer time scales, may optimize nutrient uptake according to life history strategy. Recent work demonstrates the utility of collating root nutrient uptake measurements, yet there has been very little synthesis work for tree species. This work presents a global dataset of nutrient uptake parameters in tree species. Association of these parameters with root traits was examined using the Fine-Root Ecology Database (FRED 3.0), and meta-analysis was used to evaluate the response of nutrient uptake to nutrient fertilization and other global change drivers. Finally, the sensitivity of the forest demography model FATES to nutrient uptake parameters was determined. The compiled dataset contains observations from more than 50 studies spanning more than 40 tree species. Notably, observations are strongly biased toward temperate tree species, with few observations from tropical forests. Species with acquisitive root traits, like high specific root length, exhibit greater capacity (i.e., greater V_{\max}) and affinity (i.e., lower K_m) for ammonium and nitrate uptake. Nutrient fertilization exerted a strong negative effect on both uptake capacity and affinity. A sensitivity analysis, using E3SM Land Model-FATES, reveals that simulated net primary productivity is highly sensitive to V_{\max} for nitrogen uptake, underscoring

the importance of providing new datasets for model parameterization. Overall, nutrient-enabled forest demography models are highly sensitive to nutrient uptake parameters. These parameters are highly variable in tree species but may vary predictably with environmental drivers and life history strategies.

Study of Forest Disturbance and Recovery in Puerto Rico with Field Measurements and E3SM Land Model-FATES

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Tropical cyclones are important natural disturbances in coastal tropical and sub-tropical forests. In the past three decades, Puerto Rico experienced five hurricanes that met or exceeded category 3 (i.e., wind speed greater than 178 km/h); these major storms caused severe forest structural damage and elevated tree mortality. To improve the prediction of post-hurricane forest function and structure changes, researchers used *in situ* forest measurements at the Bisley Watershed study site in the Luquillo Experimental Forest of Northeast Puerto Rico and FATES coupled with the E3SM Land Model (ELM-FATES). Numerical experiments were performed to replicate hurricane damage on forest structure including defoliation, structural-damage-induced biomass reduction, and hurricane mortality rates for the simulation period 1950 to 2017. The study compared litterfall fluxes obtained by field census and model simulation and tree biomass in terms of plant functional types (PFTs) and diameter at breast height (DBH) size classes. By constraining model parameterization with key plant trait observations (e.g., maximum rate of carboxylation or V_{cmax} , wood density, and specific leaf area), ELM-FATES can reasonably represent PFT-level, pre- and post-hurricane leaf and aboveground biomass reduction and recovery. The model–data comparison reveals that these ELM-FATES simulations tend to overestimate the number of exceedingly large DBH trees (≥ 95 cm). This bias may be associated with deficiencies in the model for representing size-related mortality or with the representation of carbon allocation relative to tree size in ELM-FATES. The parameterization that constrains mortality rates for certain DBH groups reduces the number of trees with large DBH values (≥ 95 cm). This

research addresses the importance of implementing hurricane disturbance representations in dynamic global vegetation models integrated into Earth system models.

Understanding Water and Carbon Dynamics for Improved Prediction of Tropical Tree Function and Demographics

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Understanding and modeling the carbon and water fluxes and stores of tropical trees is critical for improving predictive capacity for forest function under a changing climate. This study investigated the processes regulating plant carbon and water balance in Panama and Brazil with the goals of testing hypotheses and providing parameterization and benchmarking datasets for FATES-Hydro. Resilience of tropical forests to climate perturbations appears to be decreasing globally, with plant hydraulics playing a large role in regulating this resilience.

Hydraulic constraints on photosynthesis become increasingly dependent on vapor pressure deficit as drought worsens, leading to novel constraints on canopy gas exchange. Hydraulic traits and mortality exhibit large shifts over time at Barro Colorado Island, Panama, consistent with climate-driven changes in the most adaptive physiological characteristics. Such shifts in hydraulic traits are also observed over a large precipitation gradient in Panama, suggesting that climate drives adaptive changes in hydraulic traits. Current work is focused on providing sapflow estimates of transpiration along with additional measurements for further tests of the hydraulic mechanisms underlying survival and mortality. This work is ongoing in both Panama and Brazil. ModEx linkages to FATES-Hydro are direct through parameterization and benchmarking of the model, along with conceptual knowledge gains that are incorporated into the model.

Role of Mesoscale Convective Systems in Driving Forest Dynamics in the Amazon

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There is limited knowledge about the recurrent mechanisms driving complex tropical forest dynamics, such as tree mortality, regrowth, and associated ecosystem characteristics and processes in the Amazon. Understanding these mechanisms is critical to comprehending the current stage of forests and how they will change with future variations of forest dynamics in response to disturbance, changing climates, and extremes. The most recurrent modes of tree mortality in the Amazon are uprooted and broken trees, which are largely associated with strong winds produced by severe convective processes. As a result, tree mortality by winds, known as windthrows, is becoming a growing area of research. Using a ModEx approach, researchers found that windthrows have a preferential direction (westward), coincident with the preferential movement of mesoscale convective systems in the Amazon. Intense convection is a predictor of windthrows and winds higher than 12 m/s can produce broken trees. This study also shows that trees are sensitive to an increase in windthrows, with the western Amazon being the most sensitive region. Vegetation regrowth after windthrows is faster in the Western Amazon than in the Central Amazon and windthrows display a spatial pattern of occurrence. Furthermore, windthrows have increased with time and show a shift toward the western Amazon. A work in progress is the nexus between inventory plots that enable *in situ* measurements of tree mortality and remote sensing data that enable regional assessments of this mortality. However, both study types are concluding similar results, mostly regarding the increase in tree mortality and its shift. Importantly, windthrows as a driver of tree mortality are not currently included in Earth system models. Future work will include development of a wind disturbance and mortality mechanism into FATES and simulations of convective characteristics responsible for windthrows using E3SM.

Remote Sensing-Based Estimates of Aboveground Biomass Time in Tropical Vegetation

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Tropical forests represent the world's largest live carbon sink and therefore play a critical role in sequestering carbon that would otherwise contribute to climate change. Estimating and monitoring the amount and dynamics of carbon stored in tropical forests greatly adds to understanding the behavior and stability of this critical carbon sink. To develop continuous, accurate, and high-resolution estimates of aboveground biomass (AGB) in tropical forests, researchers leveraged and fused remote sensing observations of structural complexity from the Global Ecosystem Dynamics Investigation project (GEDI) with canopy surface reflectance properties from Sentinel-2 satellite maps. GEDI uses space-borne lidar to measure forest structure and predict AGB between 51.6°N and 51.6°S latitudes, but GEDI is expected to be active on the International Space Station for a relatively short period of time of about three and a half years. The research team seeks to extract the relationship between vegetation structural properties and canopy spectral properties using two rich data sources to enable seasonally varying estimates of AGB using multi-spectral images from Sentinel-2, which are expected to have continued availability beyond the operational span of GEDI. The study focused on tropical vegetation in Costa Rica. Data were collected monthly for ten high resolution (10 m or 20 m) bands from Sentinel-2 from 2019 to 2022. Reflectance data were filtered for noise and clouds and temporally gap-filled using polynomial regression. GEDI Level 4A footprint-level AGB measurements and GEDI Level 2A footprint-level observations containing canopy height profiles were also collected. Level 4A data were used to train an ensemble of regression models: random forest, extreme gradient boosting, and a convolutional long short-term memory (LSTM) neural network to estimate AGB using Sentinel-2 reflectances. All models were hyperparameter tuned using fourfold spatial cross-validation with root mean squared error as the scoring metric. The results show that decision-tree-based modeling techniques appear ineffective, while LSTM is capable of producing more accurate AGB estimates from multi-spectral images.

Nutrient Dynamics in a Coupled Terrestrial Biosphere and Land Model (ELM-FATES)

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Researchers present a representation of nitrogen and phosphorus cycling in the vegetation demography model FATES within the E3SM Land Model (ELM-FATES). This representation is modular and designed to allow testing of multiple hypothetical approaches for carbon-nutrient coupling in plants. The model tracks nutrient uptake, losses via turnover from both live plants and mortality into soil decomposition, and allocation during tissue growth for numerous size- and functional-type-resolved plant cohorts within a time-since-disturbance-resolved ecosystem. Root uptake is governed by fine root biomass. The research team hypothesized a proportional-integral-derivative controller to allow plants to dynamically vary their fine root carbon allocation in order to balance carbon and nutrient limitations to growth. The sensitivity of the model was tested to a wide range of parameter variations and structural representations and in the context of observations at Barro Colorado Island, Panama. A key model prediction is that plants in the high-light-availability canopy positions allocate more carbon to fine roots than plants in low-light understory environments, given the widely different carbon versus nutrient constraints of these two niches within a given ecosystem. This model provides a basis for exploring carbon-nutrient coupling with vegetation demography within Earth system models.

Soil Texture has a Large Impact on Vegetation Dynamics Simulated by ELM-FATES

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Soil texture is an important factor influencing patterns of vegetation structure through its influence on soil water dynamics and water availability. However, characterization of soil texture heterogeneity impacts on vegetation dynamics in Earth system modeling has been elusive. To fill the gap, researchers started simulations at BIONTE, a plot within a long-term forest dynamics experiment in the central Amazon Forest using the land component in E3SM, known as ELM, and FATES. The model accounts for tropical trees and shrubs. Model configurations include lateral flow and macropore diversion of precipitation. Based on the results from short-term spinup simulations, researchers observed that (1) the fraction of shrub leaf biomass in tree/shrub assembly decreases with sand content in the soil, especially when sand content is greater than 90%, which is contrary to the observations and (2) when accounting for macropore flow parameterized based on root biomass, shrub fraction increases with sand content when sand content is less than 90%. Longer-term spinup and further investigations are planned to confirm, analyze, and understand the findings.

Pan-Tropical Calibration of Demographic Rates and Forest Structure in E3SM Land Model-FATES

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Observations from forest plots show important differences in aboveground woody productivity, biomass, and turnover of forests across continents, and how these dynamics are changing through time. These patterns are not well captured by the current generation of Earth system models. Researchers compared global simulations of the vegetation demographic model E3SM Land Model-FATES (ELM-FATES)

to ground observations of aboveground biomass and carbon turnover from Galbraith et al. (2013), and size-dependent aboveground woody productivity (AWP) and mortality from Piconiot et al. (2022). ELM-FATES with its current default parameters has a high AWP bias across much of the tropics, despite reasonable gross primary production, suggesting potential biases in the plant respiration scheme. The default respiration scheme based on Ryan (1991) was compared with a respiration scheme based on Atkin et al. (2017) to assess parameter sensitivity related to maintenance respiration. Increasing maintenance respiration or using the Atkin respiration scheme both reduced AWP to be more in line with observations. Ensuring that productivity and mortality match observations is essential to correctly modelling carbon exchange between land and atmosphere.

Assessing the Risk of Hydraulic Function Failure for Tropical Forests Under Future Climate Changes

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Tropical forests play a critical role in regulating regional and global climates. However, recent drought-induced mortality in tropical forests suggests possible thresholds beyond which communities face the risk of widespread mortality. Modeling plant physiological response to drought is crucial to accurately forecast tropical forests and their carbon storage.

Hydraulic function failure in xylem due to embolism and dehydration, resulting from both water stress in the soil and high vapor pressure deficit in the air due to warming, is a crucial avenue for future mortality. A diverse set of plant hydraulic traits determine a plant's water use strategies. Future droughts may disproportionately impact functional strategies that avoid drought through investments in greater water access or storage or tolerate it through investments in increased water stress resistance. Using 1,000 ensembles of hydraulic and growth traits, researchers parameterized a

plant hydrodynamic model within FATES coupled to the land surface model within E3SM for the forests of Barro Colorado Island, Panama. This model was calibrated against observational data from Barro Colorado Island to constrain plant hydrodynamic, carbon, and water fluxes. These ensemble parameterizations were then used under multiple climate scenarios to assess the risk of hydraulic failure and resulting mortality. Drastic increases were observed in the mean number of months in which plant species faced risk of hydraulic failure (>60% loss of stem hydraulic conductivity). However, the likelihood of potential hydraulic failure was highly trait dependent, with some functional types experiencing no increase in mortality. Researchers further analyzed the traits that make plant functional types more vulnerable to hydraulic failure. The results suggest the critical importance of considering hydraulic failure risk in simulating regional carbon cycles in tropical forests.

Virtual

Nutrient Budgets Across Pantropical Environmental and Disturbance Gradients

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As nutrient resource availability can moderate tropical forest demography, function, and recovery trajectories following disturbances and environmental changes, the carbon, nitrogen, and phosphorous nutrient-enabled FATES model (FATES-CNP) under development by Ngee-Tropics will provide a more accurate representation of nutrient controls on demographic rates and structure, and of carbon and water cycling in tropical forests. FATES-CNP will improve predictions of how primary nutrients (e.g., nitrogen and phosphorus) constrain tropical forest responses to disturbances and environmental changes throughout the 21st century. To predict how nutrient budgets and the relationships between ecosystem nutrient budgets and net primary productivity vary across pantropical environmental and disturbance gradients, researchers integrate observational and experimental plot-level data from forest sites, including those from the Global Ecosystem Monitoring network, at various successional stages spanning nutrient, climate, and

disturbance gradients into the calibration and validation of FATES-CNP. Simultaneously considered were changes in carbon and nutrient budgets, disturbance regimes, and plant functional diversity within the surveyed tropical forests. Work is ongoing at the Manaus ZF-2 research station to quantify: (1) carbon and nutrient stocks in the leaf and wood pools of generalist and specialist species and their surrounding soil pools in habitats spanning a soil texture and nutrient gradient; (2) the temporal dynamics of leaf litter production, nutrient retranslocation, and phenology in pioneer and non-pioneer species varying in wood density; and (3) throughfall and precipitation nutrient inputs in forests affected and unaffected by logging. Preliminary results indicate that nutrient generalist and specialist species occur in plateau and valley soils showing a wide range in sand, clay, total carbon and nitrogen, and available phosphorus concentrations. Across all species, wood carbon and nitrogen concentrations varied from 42.4 to 66.7% and 0.16 to 0.51%, respectively. Phosphorus varied from 0.03 to 0.15 g/kg with a two-fold difference in mean wood phosphorus but no difference in mean wood carbon and nitrogen between valley and plateau species. Future work will quantify the relationship between net primary productivity, nutrient uptake, and resorption across nine old growth and logged lowland wet tropical forests in Sabah, Malaysian Borneo. This pantropical data synthesis will elucidate how nutrient use traits relate to plant functional composition and community dynamics across pantropical sites and gradients, emergent signals of disturbances in nutrient budgets, and how nutrient budgets modulate recovery trajectories following disturbances and drought stress.

Virtual

Tropical Tree Water Availability and Sourcing

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As the global climate warms, tropical forests increasingly experience extreme heat and recurrent drought conditions, which can lead to declining growth rates and mortality

under extreme conditions. Spatial patterns of soil water availability and plant water sourcing depth, which depend on rainfall, soil texture, and topography, are important for maintaining tree function during drought. Trees employ hydraulic strategies to combat drought, including stomatal regulation, stem water storage, drought-deciduousness, niche positions on the landscape, and deep rooting. Strong evidence suggests that hydraulically vulnerable, yet deeply rooted species are less sensitive to drought, which is reflected in potentially high growth and low mortality following drought events. Rooting depth can be inferred through analysis of stable water isotopes in precipitation, ground water, soils, and tree xylem. To understand the depth of tree water sourcing across the hyperdiverse tropics, researchers assessed stable isotopes during seasonal drought in dozens of species across wood-density and life-strategy spectra of old-growth forests in Panama and Brazil. To understand water availability, researchers deployed sensors for soil water content and soil water potential across the topographic gradient of each field site. Root distribution and structural and hydraulic traits were also assessed to investigate tree level drought strategies. Data will be used to model water availability and extraction patterns and to link plant water sourcing depth to other functional plant traits to enable scaling. Results from the upland K34 tower in the central Amazon Forest indicate that a vast number of fine roots are in the upper soil, with 45% in the upper 5 cm. However, observations from the K34 soil pit revealed roots growing at depths up to 10 m, indicating some species are accessing these deep soils. During a month-long drought, upper soils dried toward the wilting point and water extraction shifted to deeper layers. An analysis indicated that the upper 2 to 3 m could sustain evapotranspiration demand. New soil water measurements across the K34 topography indicate differential rates of soil drying and water availability, and thus differential tree hydraulic stress during drought.

Water stable isotope samples are currently under analysis to assess species-trait assemblages capable of accessing deeper water. This ongoing work is poised to leverage data collection during the next El Niño event, forecasted for 2023 to 2024. Future measurements of soil water availability and tree water sourcing are planned pantropically, including in Malaysia.

Virtual

Exploring the Dominant Roles of Vapor Pressure Deficit and Soil Moisture on Vegetation Productivity Using Explainable Machine Learning

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With the increasing frequency and severity of droughts projected under future climate scenarios, the impact of drought on vegetation productivity is expected to intensify. Drought stress on ecosystem production is commonly characterized by low soil moisture (SM) and high atmospheric water demand (i.e., vapor pressure deficit; VPD). The relative dominance of VPD versus SM on vegetation production is still debatable. This study presents an explainable, machine-learning approach to disentangling the dominant role of VPD and SM in vegetation gross primary production across global ecosystems, with a particular focus on tropical regions such as the Amazon basin, using multisource datasets. The findings reveal that, globally, vegetation productivity in most landscapes is dominated by SM rather than VPD. Moreover, 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 E3SM, with vital implications for understanding global water, carbon, and energy cycles in the face of climate change.

Virtual

Global Patterns in Forest Allocation of Carbon to Reproduction

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The allocation of net primary productivity to reproduction in trees (e.g., flowers, fruits, and seeds) influences forest function through a tradeoff with growth and by being a necessary driver of recruitment. Recent evidence suggests that carbon allocation to reproduction (RA) may increase significantly with temperature and precipitation, may be greater on fertile soils in tropical forests, and may differ across successional states. However, common model parameterizations assume RA is constant across climatic, edaphic, and successional gradients, potentially biasing predictions. Researchers used a novel proxy for RA constructed from litterfall records to estimate differences in RA across forest sites globally and asked: (1) how ecosystem-level RA varies within and across biomes and (2) to what extent variation in RA is explained by climate (e.g., mean annual precipitation and mean annual temperature) and stand-level characteristics (e.g., soil and successional state). Researchers collected 1,520 observation-years of forest leaf and reproductive litterfall fluxes from 550 sites that span the forested continents. A Mann-Whitney nonparametric test was used to detect differences across biomes and general linear mixed effects models were used on transformed data to quantify continuous relationships with climate and site characteristics. Mean RA ranged from 0.11 ± 0.012 in boreal forests to 0.14 ± 0.005 in tropical forests (0.13 ± 0.005 in temperate forests), representing a 27% difference. Differences in RA across tropical and boreal forests were statistically significant (Mann-Whitney, $p < 0.001$). Globally, evidence exists for a non-linear, concave down relationship between RA and temperature, with a peak at $\sim 20^\circ\text{C}$. Researchers also found a significant negative relationship between RA and precipitation in the tropics ($p < 0.001$) but no significant relationship with precipitation in other biomes. The results suggest weaker relationships between RA and temperature and precipitation gradients than previously reported and suggest additional drivers should be examined to explain variation in reproductive allocation.

Science Focus Areas

Carbon Emissions from a Whole-Soil Warming Experiment Are Not Attenuated in the Long-Term

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By the end of the 21st century, global mean surface temperatures are projected to increase by 2.6–4.8°C, relative to 1986 to 2005, under a Representative Concentration Pathway of 8.5. Soil temperatures are projected to increase at a similar rate to air temperatures, both at the near-surface (~1 cm) and at depth (100 cm; Soong et al. 2020). This means that soil carbon in deeper soil layers, which on average cycle on centennial to millennial timescales, can become increasingly vulnerable to microbial decomposition. Since the subsoil (>20–30 cm) stores a large proportion of soil carbon in the top meter, this depth response can have significant consequences for terrestrial carbon emissions to the atmosphere.

In 2013, researchers established a whole-soil warming experiment at Blodgett Experimental Forest, a temperate forest comprising a thinned, 80-year-old stand of mixed conifers. The top meter of the soil profile was warmed by 4°C using heating rods installed 2.4 m into the soil around 3 m diameter plots, with surface heating cables buried at 5 cm depth at radii of 0.5 and 1 m. In the first five years of warming, carbon dioxide (CO₂) respiration increased 30% from decomposition throughout the entire soil profile (Hicks-Pries et al. 2017; Soong et al. 2021). In the subsoil, warming shifted soil organic matter toward more decomposed material and decreased microbial abundance (Ofiti et al. 2021; Zosso et al. 2021). The effects of warming can be large in the initial phase of disturbance and attenuate over time due to acclimation or a decrease in substrate availability for the microbial response. Thus, long-term soil warming experiments are crucial to inform Earth system models and avoid over- or underestimating soil carbon loss based on the initial warming response.

After almost a decade of warming, researchers have found that the mean annual CO₂ flux ratio (heated/control) has not significantly changed; from 2014 to 2021 it averaged between 1.2–1.4, meaning respiration in heated plots was 20–40% higher than in control plots. The CO₂ response to warming has not subsided overtime, despite some changes

in carbon substrate stocks, and support long-term projections of soil carbon loss with warming.

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Combining Experimental Warming and Environmental Gradients to Elucidate Continuous and Interacting Drivers of Soil Response to Warming

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Grassland ecosystems comprise 40% of the global ice-free land surface area and store up to a third of terrestrial carbon. Unlike most ecosystems, nearly all the carbon in grasslands is stored belowground, making the response and management of their soil carbon cycling crucial in a warmer world. Experimental warming in grasslands stimulates soil carbon fluxes, but the response magnitude varies significantly among studies. Ecosystem responses to warming can be difficult to assess due to large or unmeasured spatial and temporal heterogeneity and limited numbers of field replicates (Kreyling et al. 2018). To address some of these issues, scientists are setting up a new whole-soil warming experiment in a California coastal grassland in Point Reyes, where they will heat the top meter of soil by 3°C and 6°C relative to control plots. Soil will be warmed using 22 heating rods in a 4 m diameter circle and a central rod all installed 2.4 m deep in the soil, plus three circular surface heating cables buried at 5 cm at radii 0.45, 1.0, and 1.75 m. Extensive multidisciplinary site characterization was conducted to better understand the spatial heterogeneity of the site. The small

elevation gradient has three distinct zones (e.g., upslope, midslope, and downslope) that are shaped by vegetation, hydrological, and pedological properties. Twenty-four strategically placed plots grouped into eight blocks span the three zones along this gradient. Soil carbon dioxide flux varies spatially and temporally across the gradient. In late winter and early spring, when plant activity is low and soil moisture is at its maximum, soil flux is lower downslope relative to the other zones, due to highly saturated soils. As the growing season progresses, soil flux increases across the site reflecting enhanced root respiration from higher plant productivity. As the soil becomes less saturated downslope, soil flux rates more than double relative to the upslope and midslope zones, where normalized difference vegetation index and soil moisture values are lower and plants senesce earlier in the season. This research will capitalize on the vegetation and soil moisture gradient at the site (1) to better elucidate interacting environmental drivers and their response to whole-soil warming and (2) to improve the overall prediction success given the high spatial heterogeneity, which is common in ecological experiments.

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A Larger than Expected Role for Calcium in Binding Soil Organic Carbon in Acidic Soils: Results from the Belowground Biogeochemistry Science Focus Area

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Past research on the retention and accumulation of soil organic carbon (SOC) has focused on its biogeochemical interactions with iron (Fe) or aluminum (Al), largely overlooking a role of calcium (Ca). Recent studies have demonstrated a strong link between Ca and SOC in a range of soil types (Rasmussen et al. 2018; Yang et al. 2020), but the current conceptual model limits the role of Ca on SOC to soils with carbonates and a basic soil pH (pH > 6; Rowley et al., 2018). Working with the whole-soil warming sites of the Belowground Biogeochemistry SFA, researchers combined classical characterization methods with synchrotron-based spectromicroscopy to analyze Ca-SOC interactions in soil

samples taken from the Point Reyes National Seashore and Blodgett Experimental Forest warming sites (soil pH 3.8–5.3) in California.

Both the Ca and SOC content were high in samples at Point Reyes and were correlated in multivariate analyses of the project's classic characterization dataset. Calcium K-edge X-ray absorption near-edge structure data revealed that Ca was predominantly associated with organic matter at the site. Additionally, scanning transmission x-ray microscopy analysis from both Blodgett Forest and Point Reyes showed that Ca had a strong spatial correlation with carbon (C). Characterization of the SOC associated with Ca revealed spectral features consistent with C that had a higher proportion of aromatic and phenolic C, relative to C associated with Fe. These features in the C near-edge X-ray absorption fine structure spectra were observed in samples obtained from up to 70 cm depths at both sites. This work thus suggests that the Ca-C association observed from bulk soil analyses arises from the preservation of more plant-like products, even at depth in acidic grassland and forest soils developed on different parent material. These findings now challenge existing paradigms that these Ca-mediated processes are only found in soils with a pH > 6.5. Incubations are underway to connect the Ca-association processes to impacts on total respiration.

Rasmussen, C., et al. 2018. "Beyond Clay: Towards an Improved Set of Variables for Predicting Soil Organic Matter Content," *Biogeochemistry* **137**(3), 297–306. DOI:10.1007/s10533-018-0424-3.

Rowley, M. C., et al. 2018. "Calcium-Mediated Stabilisation of Soil Organic Carbon," *Biogeochemistry* **137**(1), 27–49. DOI:10.1007/s10533-017-0410-1.

Yang, S., et al. 2020. "Lithology Controlled Soil Organic Carbon Stabilization in an Alpine Grassland of the Peruvian Andes," *Environmental Earth Sciences* **79**(2), 66. DOI:10.1007/s12665-019-8796-9

Resolving the Influence of Ice Wedge Polygon Formation and Geomorphology on the Carbon and Nitrogen Stocks of Arctic Coastal Lowland Soils

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Ice-wedge polygons (IWP) are ubiquitous, patterned ground features throughout Arctic coastal plains and river deltas. At the local scale, researchers are investigating the

hypothesis that progressive ice-wedge expansion creates a natural developmental evolution from flat- to low- to high-centered IWPs that influences the degree of cryoturbation and soil formation, both of which impact the distribution of soil organic carbon (OC) and total nitrogen (TN) stocks. Further, variations in OC and TN stocks at the landscape to regional scale are affected by polygon geomorphology (trough vs. center), polygon size, the spatial distribution of polygon types (i.e., flat-, low-, and high-centered IWPs), and soil parent material. To investigate these hypotheses, researchers sampled 9 to 12 IWPs (three to four of each type) formed on three contrasting parent materials typical of the Arctic Coastal Plain of Alaska: (1) glaciomarine sediments dominating the thaw-lake terrain near Utqiagvik, (2) fluvial deposits on terraces of the Sagavanirktok River, and (3) the extensive surficial material classified as coastal plain mixed deposits near Milne Point. For each of the 30 IWPs, researchers quantified the distribution of OC and TN stocks across entire two-dimensional polygon profiles to depths up to 3 meters by extensively sampling the cross-section stratigraphy of soil horizons and ice wedges of transects spanning from trough center to trough center. Initial results indicate that OC stocks in troughs are consistently and substantially lower than those of polygon centers due to the significant subsurface volumes occupied by ice wedges. In polygon centers, OC stocks differed among parent materials. However, within parent materials, a similar pattern of increasing OC stocks from flat- to low- to high-centered IWPs lends support to the hypotheses linking OC stocks to the natural evolutionary cycle of IWP development and soil formation. Ultimately, the data generated by these studies will be used to investigate whether accounting for the fine-scale geomorphology and distribution of different polygon types can provide more accurate geospatial estimates of soil OC and N stocks for coastal landscapes dominated by IWPs. The spatially and vertically resolved data is also expected to inform and constrain the parameterization of process models being developed to simulate regional responses to future climatic conditions.

Quantifying Spatial and Vertical Variations in Soil C:N Relationships for the Permafrost Region Using Machine Learning

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Soil property ratios are often used to characterize soil organic matter composition and other measures of soil quality. However, mapping and spatial interpretation of soil property ratios is challenging, with no set standard, particularly for the heterogeneous profiles of permafrost-affected soils. Two different approaches—direct and indirect mapping—can be used. For direct mapping, property ratios determined for each soil observation are used to predict their distribution within the landscape. With indirect mapping, each property is predicted independently across the landscape, and the ratio of the resulting two maps are then used to calculate the predicted ratio for each map pixel. Researchers used observations of soil organic carbon (C) and total nitrogen (N) stocks in Alaska to investigate which mapping approach best captures the distribution of soil property ratios for cold region soils. The specific objectives were to: (1) evaluate which approach best captures the distribution of soil C:N ratios at high spatial resolution for a selected latitudinal transect in Alaska and (2) identify which environmental covariates are important predictors of the spatial and vertical variation of soil C:N ratios within the study area. Three machine-learning approaches (cubist, Random Forest, and extreme gradient boosting) were compared. Maps of predicted soil C:N ratios were generated at a spatial resolution of 34 m for three depth increments within the surface meter. Overall, indirect mapping with Random Forest performed best at depths of 0 to 30 cm ($R^2=0.27$, RMSE=4.88) and 30 to 60 cm ($R^2=0.20$, RMSE=7.57), whereas direct mapping with cubist performed best at 60 to 100 cm ($R^2=0.36$, RMSE=5.92).

Even though temperature was the most dominant predictor overall, terrain attributes were most important at finer scales. Conversely, parent material was the least important predictor. Both mapping approaches, however, underpredicted low observations and overpredicted high observations due to the relatively low sampling density and the uneven distribution of observation locations and their C:N values within the study area. Knowledge gained from this work will inform

ongoing efforts to map soil C:N ratios, as well as soil organic C and N stocks, for the state of Alaska at a spatial resolution of 34 m. Ultimately, the maps will be useful for informing and benchmarking large-scale land surface models.

Investigating Microbiome Contributions to Soil Organic Matter Degradation Across a Boreal Forest to Arctic Tundra Gradient

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The degradability of organic matter (OM) held in permafrost-affected soils is expected to affect the rate of carbon (C) mineralized, mobilized, and released from these soils in response to global warming. While many factors influence the degradation of OM in permafrost-region soils (e.g., temperature, C species, organomineral associations, water content, redox conditions, pH, and soil texture), warming of these soils is expected to enhance heterotrophic respiration rates and the mineralization/loss of C stocks currently held in them. Previous studies indicate that a soil's total organic C (TOC) concentration can often reasonably predict C loss as carbon dioxide (CO₂), but unexplained variation remains. The purpose of this study is to evaluate the decomposability of permafrost and active layer soil horizons across a large latitudinal and vegetation gradient (~500 km) from Fairbanks, AK, to north of the Brooks Range. Horizon-specific samples of the full soil profiles (to a depths of 1 m) were collected, stored frozen, freeze-dried, homogenized through a 2-mm sieve, and then subsampled for analysis of the native microbial community composition and TOC. Additional aliquots of these soils are being evaluated for loss of CO₂-C when subjected to warming conditions in an aerobic manipulative bioassay-incubation (rewetting to uniform matrix potentials). To compare the decomposability of OM present in these soils with potential response predictors, researchers initiated analyses of the relationships between respiration rates during the first two months of incubation and several covariates including TOC, microbial community structure and diversity, and their combination. A clear difference was observed in respiration rates (mass basis) and time to peak respiration between organic and mineral horizons, suggesting some differences in OM degradability between these horizon types. Inclusion of microbial parameters, in addition to TOC, is hypothesized

to improve predictive models of C loss from permafrost-affected soils because strong divergence is expected in microbial community structure between horizon types within different soil profiles, which might influence mineralization potentials. The data generated here will be used to: (1) inform future predictive models of soil C loss for the permafrost region and (2) guide procedures for assessing the spatiotemporal variability of both microbial and C species diversity in warming permafrost-affected soils.

Virtual

Oak Ridge National Laboratory's Terrestrial Ecosystem Science SFA: A 2023 Overview

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Understanding fundamental responses and feedbacks of terrestrial ecosystems to climatic and atmospheric change is the aim of the Oak Ridge National Laboratory's (ORNL) Terrestrial Ecosystem Science (TES) SFA. The proposed research efforts of the ORNL TES SFA seek to provide answers to the following overarching question: How vulnerable to climate change are carbon (C) stores of eastern North American ecosystems, and what are the implications for C–climate feedbacks? The TES SFA focuses on eastern United States ecosystems vulnerable to water cycle and energy changes whose impacts are highly uncertain in Earth system models. Proposed science includes manipulations, multidisciplinary observations, database compilation, and fundamental process studies integrated and iterated with modeling activities. The dominant manipulation is the SPRUCE experiment testing responses to multiple levels of warming at ambient and elevated CO₂ for a *Picea-Sphagnum* peatland ecosystem. Long-term observations of ecosystem function at the Missouri Ozarks AmeriFlux (MOFLUX) eddy covariance site provide the opportunity to characterize ecosystem response to dominant hydrologic limitations. Further process-level work occurs at smaller scales and aims to improve mechanistic representation of processes within terrestrial biosphere models by furthering scientific understanding of fundamental ecosystem functions and their response to environmental change. The TES SFA integrates experimental and observational studies with model building, parameter estimation, and evaluation to yield reliable model projections. This integrated model-experiment

approach focuses on improving the E3SM Land Model (ELM) and fosters enhanced, interactive, and mutually beneficial engagement between models and experiments.

Highly Dynamic Versus Monthly Community Net Carbon Dioxide and Methane Flux Observations for SPRUCE Warming by Elevated Carbon Dioxide Experiment: Comparing Integrated Data

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The net flux of carbon dioxide (CO₂) and methane (CH₄) from the intact peatland community being studied in the SPRUCE experiment is a critical component of the ecosystem carbon budget and a controlling variable that determines the performance of the ecosystem as a landscape source or sink of carbon. In the first 6 years of SPRUCE operations, net flux of these two gases were collected across warming treatments at approximately monthly intervals throughout the active season to capture seasonal dynamics of flux and the relative balance between CO₂ and CH₄ emissions. These data were integrated over time based on half-hourly environmental data correlated with the observed fluxes and used as a primary input for calculated net ecosystem carbon exchange. Upon the advice of the SPRUCE Advisory Panel members, and with DOE financial support, automated flux chambers capable of subhourly observations of flux were deployed to the SPRUCE treatment plots in 2022 and contrasted with occasional manual, large-collar flux observations. Comparative observations for 2022 showed comparable CO₂ and CH₄ flux magnitudes between approaches, but also provided clear evidence of transient spikes of CH₄ flux often missed by the periodic manual flux observations. This analysis will present these data and integrated flux estimates using each approach and propose improved mechanistic representations for net greenhouse gas fluxes necessary to include the dynamic nature of episodic CH₄ release from the peatland.

Organic-Matter Decomposition Responses to Whole-Ecosystem Warming in a Northern Peatland

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Peatlands are carbon-rich ecosystems. Globally, peatlands cover only 3% of the Earth's land surface but store 30% of terrestrial carbon. Peatlands in northern environments accumulate carbon over time because saturated, cold, and acidic conditions result in slow organic matter decomposition rates. However, northern peatlands are vulnerable to climate change, with warmer temperatures expected to accelerate decomposition rates. Within the SPRUCE project, multiple organic matter decomposition experiments are being conducted to better understand the responses of decomposition to warming. Researchers used a litterbag approach to measure decomposition rates of six litter types (e.g., spruce needles and fine roots, Labrador tea leaves and fine roots, and two Sphagnum species). A peat-ladder approach was also used to measure decomposition rates of peat soil at 10 cm depth increments (from 0–40 cm). After multiple years of incubation (6 years for the plant tissues and 3 years for the peat soil), results showed little effect of warming on decomposition rates.

While Labrador tea leaves and fine roots decomposed faster with warming, the other types of plant litter and peat soils did not respond to warming. These decomposition studies were conducted in shallow peat, limiting understanding of decomposition responses at deeper depths. Further, because decomposition rates are slow in peatlands, litterbag and peat-ladder approaches that integrate decomposition rates over multiple years make it difficult to understand seasonal and interannual variation and elucidate environmental drivers. Therefore, the third approach used cotton strips, which are a labile carbon source (95% cellulose), to examine decomposition responses to warming seasonally (winter, summer) and throughout the depth profile (surface to 1.3 m depth). Cotton strips (1.37 m long, 2.5 cm wide) were deployed into peat seasonally for 5 years. Results showed strong positive responses of organic matter decomposition to warming but only at depths >35 cm. At shallower peat depths, soil moisture was a more important factor, with faster decomposition rates when peatland water level was

high. The cotton strip results suggest that soil moisture may be a more dominant factor affecting organic matter decomposition than temperature in near-surface peats, thus explaining the general lack of warming response in the litterbag and peat-ladder studies. These findings suggest that the direct (warming) and indirect (drying) effects of temperature on decomposition should be incorporated into models examining future climate change impacts on peat-land carbon cycling.

Plant Roots in Boreal Peatlands Under Whole-Ecosystem Warming and Elevated Carbon Dioxide Track Nutrients, Not Water

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Peatlands cover less than 3% of the global land surface but store more than one third of global soil carbon in deep deposits of peat. The interplay between the rooting depth distribution of peatland plants and peat biogeochemistry can impact peat accumulation but is understudied. Furthermore, climate change-elevated carbon dioxide (CO₂) and warming can alter the depth at which roots are found in the peat profile. Previous work in uplands has shown that elevated CO₂ tends to increase rooting depth distribution. Additionally, rising temperatures can increase evapotranspiration, depressing water table levels in saturated peatlands, possibly expanding the depth of oxic peat available to exploration by plant roots. In contrast, warming-induced mortality of Sphagnum mosses at the peat surface and corresponding increases in available nutrients may drive plants to allocate more of their roots in shallower portions of the peat profile. Peatlands comprise a number of co-occurring plant functional types with differing strategies for water and nutrient acquisition. Roots are predicted to grow deeper with elevated CO₂ and higher temperatures (via depressed water tables). Alternatively, increased nutrient availability in surface peat at higher temperatures may lead to shallow roots. These responses are predicted to be strongest in the plant functional types with the highest growth rates.

These hypotheses were tested in the SPRUCE experiment, a whole-ecosystem warming (WEW) and elevated CO₂ experiment occurring in an ombrotrophic boreal bog in northern MN. WEW treatments ranging from 0 to +9°C above ambient temperatures and increasing in 2.25°C steps were initiated in 2015. These WEW treatments are crossed by ambient and elevated (+500 ppm above ambient) CO₂, resulting in a total of ten treatment plots and two untreated control plots. Rooting depth distributions were estimated

from images collected at 3+ time points annually from minirhizotron tubes between 2018 to 2021. Elevated CO₂ did not lead to deeper root distributions, nor did plant functional types with high growth rates respond more strongly than others. Higher WEW treatments led to shallower root distributions under ambient, but not elevated, CO₂, matching patterns in nutrient concentrations in surface peat. In contrast, the water table uniformly declined with WEW across CO₂ treatments. Thus, researchers attribute these differential responses of rooting depth distribution to WEW at differing CO₂ to shifts in nutrient concentration and not changes in the height of the water table.

Microbial Changes with Depth, Treatment, and Time in the Northern Minnesota SPRUCE Experiment

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Peatlands store one third of all global terrestrial organic matter and are thus especially important to understand in response to changing climatic patterns. To understand how peatlands may respond, the SPRUCE experiment in northern Minnesota has applied whole-ecosystem, above- and belowground warming ranging from +0° to +9°C above ambient since 2015. Part of these efforts involves investigating changes in microbial communities within peat in the SPRUCE experimental plots with depth and years of warming in the acrotelm and catotelm peat using metagenome assembled genomes (MAGs) resolved via shotgun metagenomic approaches. Over the course of three sampling years (2015, 2016, and 2018), each encompassing multiple depth increments (10-20, 40-50, 100-125 and 150-175 cm), scientists have recovered approximately 800 medium- and high-quality dereplicated MAGs across the SPRUCE treatment enclosures. Overall microbial community composition and MAG alpha-diversity show strong depth stratification, likely primarily driven by variation in redox conditions across the peatland depth profile. MAG communities are dominated by Acidobacteriaota that constitute >30% of MAGs recovered across samples and years, with members of Proteobacteria, Actinobacteriota, and Verrucomicrobiota composing the majority of the remainder (at 15%, 11%, and 7% respectively). Identified methanogens also vary

with depth but peak in the 40–50 cm increment and are dominated by MAGs similar to *Candidatus Methanoflorens stordalenmirensis* (rice cluster II) that are often reported as important in other diverse systems but remain uncultured to date. Within depths approximately 100 MAGs were identified whose abundance was significantly correlated with temperature across temperature treatments, although the overall variance explained by warming treatments is low at around 4%. Previously published research from SPRUCE has revealed shifts in soil metabolomes and increased carbon dioxide (CO₂) and methane (CH₄) production with warming; however, in earlier years these seem to have been primarily driven by changes in recently fixed carbon (C) likely in porewater dissolved organic carbon pools, with C in CO₂ and CH₄ derived from older peat-derived pools only increasing in the most recent years. Ongoing efforts to characterize the extent of any further change over time in 2022 samples, as well as planned similar efforts for the end of the experiment in 2025, will investigate how any continued functional shifts in microbial communities may drive these and other changes in these important ecosystems.

Archival of Previously Published SPRUCE Experiment Data at ESS-DIVE: Approach, Successes, and Challenges

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Since 2017, ESS-DIVE has been archiving data from projects across the ESS program with a focus on findable, accessible, interoperable, and reproducible (FAIR) data principles. While this has improved the findability and accessibility of ESS data, a new question arose for older projects: How to best archive datasets at ESS-DIVE that have been previously published elsewhere?

This poster shows an overview of the process used by the ORNL Terrestrial Ecosystem Science SFA to archive data from the SPRUCE experiment that have been published previously. These data were published on the SPRUCE website (mnspruce.ornl.gov) and had DOIs registered through the Office of Scientific and Technical Information (OSTI) as early as 2009. One of the most significant challenges is maintaining consistent metadata across multiple platforms, including ESS-DIVE, the SPRUCE website, and OSTI's DOI record.

Furthermore, as part of improving FAIR data practices, the project is implementing ESS-DIVE's reporting formats for newer datasets while enhancing all datasets with keywords.

Also demonstrated is how the application of ESS-DIVE's data portal system brings additional visibility to data from the SPRUCE experiment.

SPRUCE Unmanned Aerial Vehicle Remote Sensing Program

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Unmanned aerial vehicle (UAV) technology bridges the gap among spaceborne, airborne, and ground-based remote sensing data. Its characteristics of light weight and low price enable affordable observations with extremely high spatial and temporal resolutions. Moreover, recently, the stability, flight duration, and load capacity of UAVs increased significantly with the development of flight control and battery technology, which enable more sensor varieties (e.g., optical sensor, LiDAR sensor, and radar sensor) to be mounted on small UAVs. These multisource, UAV-sensing data with high spatial and temporal resolutions drive new developments for environmental science. Remote sensing applications include forest mapping and management, terrain survey, biodiversity conservation, hydrological modeling, and phenology observations.

SPRUCE has been using this technology since 2019 and generated ~30 datasets that include high-resolution RGB images, infrared, normalized difference vegetation index, and multispectrum images. This poster provides an overview of the SPRUCE UAV program, collected datasets, related scientific activities, and future plans.

Forest Soils on the Edge: Partitioning and Modeling Drivers of Soil Respiration Near the Forest-Prairie Ecotone

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The Missouri Ozarks AmeriFlux site (MOFLUX) is located on the eastern U.S. prairie-forest ecotone and is subject to

periodic and seasonal droughts. Long-term measurements of total soil respiration were complemented with plots trenched to isolate heterotrophic respiration beginning in 2017, and quarterly measurements collected of texture, pH, moisture content, carbon, and nitrogen in bulk soils and in microbial biomass, and root length and mass. Scientists applied artificial intelligence and wavelet coherence analysis to determine the effects of environmental factors on 17 years of soil respiration data (2004 to 2021) including 4 years (2017 to 2021) of heterotrophic respiration. Random Forest models identified the relative importance of heterotrophic and autotrophic respiration, including soil temperature, soil moisture, leaf-area index (LAI), and time. Wavelet coherence analysis examined the timescales (e.g., daily, weekly, monthly, or seasonal) of key drivers. Results showed that heterotrophic respiration was most responsive to soil temperature at daily and seasonal timescales, while autotrophic respiration was most responsive to aboveground productivity (using LAI as a proxy) and the time of the year. Heterotrophic and autotrophic respiration had similar responses to temperature but not to LAI or time of year; therefore, these were most influential for partitioning between heterotrophic and autotrophic respiration. Soil moisture was most important to respiration on synoptic weekly-to-monthly timescales. Finally, respiration data was used to test implementations of conventional and microbially explicit soil carbon models with alternative soil moisture response functions. To do this, scientists used the multi-assumption soil carbon model developed in the multi-assumption architecture and testbed (MAAT). This model has been developed in response to the vast diversity of soil carbon models representing different combinations of process representations. MAAT is a highly modular modeling framework that can be used to probe the sources of structural and parametric model uncertainty. Using MAAT, scientists found that the choice of moisture response process representation can lead to simulated soil carbon differing by as much as 10% after a 4-year simulation.

An Efficient Data Toolkit for Uncertainty Quantification in Ultrahigh-Resolution E3SM Land Model Simulations

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<https://tes-sfa.ornl.gov>

With the development of high-resolution datasets and the availability of supercomputing, large-scale land simulation at

ultrahigh-resolution (1 km by 1 km) becomes feasible. This study presents a toolkit designed for large-scale data processing to support uncertainty quantification (UQ) in ultrahigh-resolution E3SM Land Model Simulations (uELM) simulations on massively parallel computers, such as Summit and Frontier. This study presents the first application of its data toolkit to prepare atmospheric forcing and surface properties datasets for UQ in uELM simulations over North America. The simulation domain is an 8075 by 7814 grid at a 1km by 1 km resolution. The atmospheric forcing dataset used in this study is a temporally interpolated Daymet dataset with a 3-hour interval. The total size of the forcing dataset is around 50TB, containing seven variables: precipitation, shortwave radiation, longwave radiation, pressure, temperature, humidity, and wind.

A general approach is developed to support flexible partitioning schemes (e.g., round robin, romanization, and area of interest) over the designated domain, containing 22 million land grid cells (approximately 22,000,000 km²). A new surface properties dataset (containing over 60 variables) is derived from a 0.5-degree by 0.5-degree global surface properties dataset using a nearest-neighbor approach or linear interpolation. The final surface properties data product takes about 120GB. The computational platforms used in this study include an Nvidia DGX station (a 20-core Intel Xeon processor, 250GB memory, and 2TB of SSD storage) and a (704)-node commodity-type Linux cluster (Andes) connected to 250PB parallel file system. Each node contains two 16-core 3.0GHz AMD EPYC processors and 256GB of main memory. The partition and generation of domain-dependent subsets of atmospheric forcing datasets took approximately 10 to 12 hours using 10 Andes nodes. The generation of fine-resolution surface datasets took around 20 minutes on the DGX station. Further profiling confirmed that this data toolkit is an efficient, memory-bounded application.

Optimizing the Electron Transport Chain to Sustainably Improve Photosynthesis: Insights from a New Photosynthesis Model

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Genetically improving photosynthesis is a key strategy for boosting crop production to meet rising food and fuel demands of a rapidly growing global population in a warming climate. Many components of the photosynthetic apparatus have been targeted for genetic modification for improving photosynthesis. Successful translation of these

modifications into increased plant productivity in fluctuating environments will depend on whether the electron transport chain (ETC) can support the increased electron transport rate without risking overreduction and photo-damage. At the present atmospheric conditions, ETC appears suboptimal and will likely have to be modified to support proposed photosynthetic improvements and to maintain energy balance.

Based on a new model of photosynthetic electron transport (Gu et al. 2022, 2023), this study derives photochemical equations to quantify the transport capacity and corresponding reduction level based on the kinetics of redox reaction along the ETC. Using these theoretical equations and measurements from diverse C3 and C4 species across environments obtained by Leafweb (www.leafweb.org), scientists identified several strategies that can simultaneously increase the transport capacity and decrease the reduction level of ETC. These include (1) increasing the abundances of reaction centers, cytochrome b6f complex, and mobile electron carriers; (2) improving their redox kinetics; and (3) decreasing the fraction of secondary quinone-nonreducing photosystem II reaction centers. Findings facilitate the development of sustainable photosynthetic systems for greater crop yields.

Gu, L., et al. 2023. "An Exploratory Steady-State Redox Model of Photosynthetic Linear Electron Transport for Use in Complete Modeling of Photosynthesis for Broad Applications," *Plant, Cell & Environment* **46**(5), 1540–1561. DOI:10.1111/pce.14563.

Gu, L., et al. 2022. "Granal Thylakoid Structure and Function: Explaining an Enduring Mystery of Higher Plants," *New Phytologist* **236**(2), 319–329. DOI:10.1111/nph.18371.

Improving the E3SM Land Model Photosynthesis Using Satellite Solar-Induced Chlorophyll Fluorescence and Machine-Learning Techniques

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The parameterization of key photosynthesis parameters is one of the key uncertain sources in modelling ecosystem gross primary productivity (GPP). Solar-induced chlorophyll fluorescence (SIF) offers a good proxy for GPP since it measures the actual process of photosynthesis; while machine learning (ML) provides a robust approach to model the GPP-SIF relationship. The research team trained

the Boosted Regressing Tree (BRT) and the Random Forest (RF) ML models with Greenhouse Gases Observing Satellite SIF data and *in situ* GPP observations from 49 eddy covariance (EC) towers. These trained ML GPP-SIF models were fed into the E3SM Land Model (ELM) to generate ELM-simulated global SIF estimates, which were benchmarked against satellite SIF observations with a surrogate modelling approach. Results indicated good modeling performance of the ML-based GPP-SIF relationship. The ELM model when fed with the ML GPP-SIF models also can well predict the spatial-temporal variations in SIF. The research team also found high model accuracy for the surrogate modeling. Model parameter sensitivity analysis suggested that the fraction of leaf nitrogen in the photosynthetic enzyme ribulose-1,5-bisphosphate carboxylase-oxygenase is the most sensitive parameter to the SIF; other sensitive parameters include the Ball-Berry stomatal conductance slope (*m*_{bbopt}) and the V_{cmax} entropy (*v*_{cmaxse}). The posterior uncertainty in simulated GPP was greatly reduced after benchmarking, and the model produced improved spatial patterns of mean GPP relative to FluxCom GPP. This integrated approach provides a new avenue for improving land models and using remote-sensing SIF, which can be further improved in the future with more ground- and satellite-based observations.

Virtual

Whole-Tree Dehydration–Rehydration Dynamics of Six Co-Occurring Tree Species

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Drought, a pervasive threat to plant productivity across the globe, is projected to intensify under climate change. Accurate representations of plant and ecosystem drought responses are needed for carbon cycle and climate projections to support decision-making for adaptation and risk management. Trees possess a range of traits that interact with climate to mediate water use. Yet, there are considerable knowledge gaps concerning seasonal interannual and whole-tree water status dynamics (dehydration and rehydration) of co-occurring species with different traits that comprise a plant community. This research leverages nearly two decades of weekly to bi-weekly predawn leaf water potential measurements to characterize dehydration–rehydration dynamics of 6 tree species that have a range of drought adaptations (*Quercus alba*, *Q. velutina*, *Carya ovata*,

Acer saccharum, *Juniperus virginiana*, *Fraxinus americana*) in relation to climate. Data were collected at the Missouri Ozark AmeriFlux (MOFLUX) site, which is situated in a drought-prone *Quercus-Carya* (oak-hickory) forest in the transitional zone between the Eastern Deciduous Forest and the Great Plains. This site experiences frequent seasonal physiological drought, and a broad range of conditions ranging from years with no water stress to exceptional drought. This poster reports preliminary analyses and highlights the next steps for linking water status dynamics with plant traits.

Other National Laboratory-Led Projects

Early Career

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 (C) sink and 29% of global soil C, but the stability of C in these ecosystems under a changing climate is unknown.

Recent work suggests moisture may be more important than temperature in driving soil C storage and emissions in the tropics. However, data on belowground C cycling in the tropics is sparse, and the role of moisture on soil C 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 C stocks and radiocarbon (^{14}C) values of profiles from over 40 sites spanning 12 pantropical regions. The sites represent a large range of moisture, spanning 710 to 4200 mm of mean annual precipitation (MAP) and include Alfisols, Andisols, Inceptisols, Oxisols, and Ultisols. Researchers found a large range in soil ^{14}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 ^{14}C profiles and C stocks, with smaller C stocks and younger soil C 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. Researchers are exploring the influence of controlling factors in manipulation experiments and constrained gradients of precipitation, soil type, root inputs, geomorphology, land use, and disturbance on C storage and longevity through collaborative site-specific studies.

AmeriFlux at Scale: Paving the Way to Supporting 1,000+ Flux Sites

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<https://ameriflux.lbl.gov/>

The AmeriFlux Management Project (AMP) is well on its way to supporting over 1,000 sites in the next decade, based on recent growth. The AmeriFlux network currently has over 600 sites registered, with data available for 444, and over 5,000 unique downloads since 2015. AMP offers a wide range of services to the scientific community, including technical site visits, equipment loans, calibration gases, rapid response systems, high-frequency data storage, quality assurance and quality control (QA/QC) processing, data product digital object identifiers, and standardization of flux and meteorological (flux-met) data. Researchers highlight ongoing and future efforts to keep meeting the increasing demand for AmeriFlux data services.

The AmeriFlux BASE data-processing pipeline receives flux-met data in a standardized half-hourly format from site teams. Automated QA/QC checks are executed, results are communicated to site teams via online reports, and communications and issue resolution are managed via a customized issue tracking system. The resulting data product is made available for download on the AmeriFlux website. The pipeline is continually enhanced, most recently by piloting a system for self-review QA/QC by site teams. Over 3,000 site-years of data are available to researchers and educators who can tailor their search with the updated AmeriFlux Data and Site Search webpage, which includes filters for years of data availability, data variable type, site characteristics, and more.

Starting from the AmeriFlux BASE data product and additional information about the site, the ONEFlux processing pipeline was used to create the FLUXNET data product. Key steps in the ONEFlux pipeline are: (1) gap-filling of micrometeorological, flux, and other environmental variables; (2) partitioning of net ecosystem carbon dioxide fluxes into respiration and gross primary productivity; and (3) estimation of uncertainty from the measurements and data processing steps. The AmeriFlux FLUXNET data product is available for over 75 sites. This product is fully compatible with the widely used FLUXNET2015 product

and updated FLUXNET products being generated by other regional networks.

AMP also implemented a distributed and scalable framework for site visits and training, which are increasing the number of sites assessed and enhancing community engagement. AMP has seven Rapid Response Systems that are loaned for emerging research opportunities (e.g., urban systems and disturbance). These data products and research resources are used in many different applications, such as model evaluation (e.g., International Land Model Benchmarking package; iLAMB), remote sensing validation, ecosystem research, and natural resource management.

Crossing the Boundary: The Role of Evergreen Forest Vegetation on the Bowen Ratio in the Southeastern United States

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Vegetation and atmosphere processes are coupled through complex physical, chemical, and biological interactions. These processes regulate surface–atmosphere exchanges of carbon, water, and energy, which exert strong controls over emergent weather and climate patterns and are subject to land–surface feedbacks operating across a wide range of spatial and temporal scales. This surface–atmosphere coupling is primarily governed by sensible (conductive) and latent (evaporation and transpiration) heat fluxes and associated carbon cycle processes, which are primarily regulated by plant photosynthesis and transpiration. While it is known that there are important biotic and abiotic controls on these processes, the representation of vegetation structure, function, and water and energy cycling in land–surface and boundary layer modeling is typically incomplete, which results in large model uncertainties that limit understanding of the key connections between the land and atmosphere. In this project, researchers set out to address a key driver of model uncertainty by studying biotic and abiotic controls on the Bowen ratio—the ratio between sensible and latent heat flux that describes the amount of energy transfer between the surface and atmosphere. To connect measurements to the larger forest ecosystem-scale fluxes within the southeastern United States, the team conducted research at the National Ecological Observatory Network (NEON) Talledega National Forest eddy covariance site, an evergreen forest dominated by longleaf (*Pinus palustris*) and loblolly (*Pinus taeda*) pines, with mixed oak species in

the understory. Researchers developed and instrumented 30 evergreen trees with a prototype sap-flow sensor system along an existing instrumented soil moisture gradient. The sap-flow sensors provide continuous measurements of tree water cycling within the footprint of the flux tower, allowing connection of seasonal variation in ecosystem-scale carbon, water, and energy fluxes to tree-scale transpiration. Using prototype sensors, the team identified important differences in tree sap flux across seasonal timescales, between species, and across a moisture gradient that are strong drivers of the temporal and spatial variation in the Bowen ratio.

Investigating the Carbon Dioxide Response of Secondary-Succession Forests at Duke and Oak Ridge FACE Experiments Simulated with ELM-FATES-CNP

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Anthropogenic activities have greatly impacted Earth's ecosystems via changes in land use, land cover, and changes in climate due to increased atmospheric carbon dioxide (CO₂) concentration. Rising atmospheric CO₂ drives carbon (C) fertilization which can increase vegetation biomass production and soil C. Gains in biomass and soil C slows atmospheric CO₂ growth.

Experiments have demonstrated significant gains in net primary productivity (NPP) and biomass, suggesting that interventions such as increased fertilization, CO₂ enrichment, and improved nutrient management can have positive impacts on plant growth and C sequestration in terrestrial ecosystems. Many terrestrial biosphere models have also suggested that elevated atmospheric CO₂ (eCO₂) has caused a large fraction of land C sequestration during recent decades and predict that this sequestration will continue to increase in the future. Thereby continuing to slow the pace of climate change. Another significant component of global change has been the conversion of natural forests to secondary forests and plantations. First-generation Free Air Carbon Enrichment (FACE) experiments were conducted primarily in secondary forests and plantations, such as Duke and Oak Ridge, and provide information on eCO₂, nitrogen (N), and decade-long demographic process interactions. FACE experiments indicated that the variability in the eCO₂ response is related to stand structure, nutrient limitation,

and progressive nitrogen limitation (PNL). The experiments at Oak Ridge National Laboratory (ORNL) demonstrated the evidence of PNL of the net primary production response to eCO₂.

N cycling processes are still poorly understood and represented differently among models. Understanding the interactions of availability of N for plant uptake and growth is necessary to improve predictive capabilities of models to simulate ecosystem C storage in response to eCO₂. Researchers use ELM-FATES-CNP (nutrient-enabled and size-structured vegetation demography model with C and nutrient cycling) to simulate the Duke and Oak Ridge FACE

experiments and investigate the influence of forest size structure on eCO₂ responses and their nitrogen constraints during FACE experiments in early and late successional secondary forests. The team used a C-only version of the model alongside two soil nutrient cycling hypotheses or conceptualizations that currently exist in ELM—relative demand and equilibrium chemistry approximation—modified to represent a dynamic allocation scheme that is more consistent with the data. Using the data collected at ORNL and Duke FACE experiments, the team will evaluate the various ELM-FATES simulations and investigate the coupling of nutrient dynamics and stand structure development and their influence on eCO₂.

Small Business Innovation Research/ Small Business Technology Transfer Research

Virtual

RootShape: Automated Analysis of *In Situ* Fine Root Images

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The ability to detect and measure plant features is fundamental to a host of problems in horticultural science and plant phenotyping. Observations of roots, how they grow, and how they interact with their soil environment have important scientific and commercial implications.

Though largely obscured, root features are essential for discovering how plants respond to short- and long-term

environmental changes. Measuring the growth and distribution of fine roots is important for understanding how plants derive nutrients and water from soil and relationships between plants and mycorrhizal fungi.

Images of plant root systems can be collected nondestructively without damaging or killing the plant using rhizotrons—transparent interfaces that enable imaging of soil and roots. *In situ* imaging is an area of active research. Rhizotrons and minirhizotrons—transparent tubes and associated camera and scanning systems—are examples of imaging modalities that enable *in situ* collection.

The standard approach to segmenting roots in rhizotron images is manual tracing. Manual tracing and annotation are time consuming, tedious, and are the primary bottleneck in rhizotron image analysis. Supervised learning approaches can reduce the need for manual tracing but do not eliminate it because they are unlikely to generalize across diverse experimental designs and environments.

The approach to automating segmentation and annotation utilizes differential geometry applied to digital rhizotron and minirhizotron images to recognize and filter root-like regions from background. Then a low-dimensional vectorization of these segmented regions is derived, which can be used to train a very simple classifier with limited user intervention.

WATERSHED SCIENCES

University Projects

Student

Effect of Hydrological Variations on Biogeochemical Processes Within Contaminated Stream Sediments and the Use of Uranium as a Geochemical Tracer for Recent Changes to the Sediment Redox State

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Riparian and streambed sediments are highly dynamic environments sensitive to hydrological changes in which small variations in flow regimes may result in extensive changes to the bulk redox state of the sediments. For example, intermittent stream sediments may be subjected to net influent (losing) or effluent (gaining) conditions with respect to subsurface flow, although the degree of surface and subsurface mixing varies both temporally and spatially and results in unique and shifting redox regimes. Such redox toggling makes short-term fluxes of greenhouse gases difficult to predict and long-term carbon budget estimates less accurate. In this field-based study of uranium-contaminated stream sediments, the spatiotemporal variations in biogeochemical redox processes were revealed through a combination of *in situ* semicontinuous voltametric measurements at four different depths in the sediment and *in situ* pore water depth profiling at discrete timepoints. Dissolved oxygen (DO) was consistently detected at centimeters depth at the losing reach, whereas DO was depleted within millimeters of the sediment–water interface at the gaining reach. Dissolved ferrous iron was consistently abundant in the gaining reach and often accompanied by aqueous clusters of electrochemically active iron sulfide, whose formation indicates recent or concomitant sulfate reduction. Signs of active sulfate reduction were also captured in the form of pulsing electrochemical signals of dissolved sulfides that migrated upward during the summer months. Electrochemically active soluble organic-iron(III) complexes were absent in the losing reach and ubiquitous in the gaining reach. These signals often peaked immediately below the oxic–anoxic interface and persisted at depth, possibly indicative of the dynamic recycling of iron(III). Dissolved uranium covaried with dissolved iron and orthophosphates in both locations, indicating that uranium distribution may trace dynamic redox interfaces. Storm events disrupted redox zonation by

entraining oxygenated waters deeper into the sediment at both locations and temporarily washing out reduced metabolites at the gaining reach. Contrary to the opposing electrochemical signatures and despite a tenfold difference in total dissolved iron, similar bulk aqueous ferric-to-ferrous iron ratios were observed in both systems. These findings imply common, broad-scale processes involved in iron cycling that may result from rapid, hydrologically driven redox oscillations. In a changing climate and as demand for natural resources continues, the pressure exerted on hydrologically sensitive ecosystems increases. Improved understanding of these hydro-biogeochemical dynamics may unravel the complexities of carbon remineralization and better inform carbon budgets as well as elucidate the timing and extent of greenhouse gas emissions.

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

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Belowground in the soil, microbes breakdown organic matter, releasing carbon dioxide (CO₂). Plant roots produce CO₂ also, via their metabolism. This research aims to understand how moisture inputs, such as snow and rain, influence the amount of CO₂ produced belowground in the East River watershed, near Crested Butte, CO. In June 2021, researchers instrumented four sites along Snodgrass Mountain in the two main forest types of the region, aspen and spruce/fir conifer. To date, researchers have continuous measurements of the flux of CO₂ from the soil to the atmosphere, and its primary environmental and biological drivers (soil moisture, air and soil temperature, and snowpack and plant phenology). In 2022, researchers applied a radiocarbon source partitioning approach to determine the contributions from roots and microbes to the total soil CO₂ flux during the summer months. The work is motivated by the overarching hypothesis that quantifying belowground plant and microbial processes separately, and how they are influenced by snow and rain inputs, is necessary for understanding and predicting how the belowground East River watershed ecosystems will respond to changes in the environment.

Total water inputs differed between measurement years due to winter snowfall (428 mm water in 2020 to 2021 vs. 560 mm H₂O in 2021 to 2022). Monsoon rain amounts

were similar between summers, but differed how they were distributed, with few, large events in 2021, and smaller more evenly distributed rains in 2022. These differences in precipitation translated into wetter June to July soils (by $0.05 \text{ m}^3 \text{ m}^{-3} \text{ VWC}$) and cooler June to September soils (by $-0.31 \text{ }^\circ\text{C}$) in 2022. Larger soil CO_2 fluxes (June to September) were observed across all sites in 2022, with an average increase of 133 g C m^{-2} . Between both years, the largest fluxes were observed at the middle elevation aspen ($377.9 \pm 132 \text{ g C m}^{-2}$) and conifer ($421.13 \pm 74 \text{ g C m}^{-2}$) stands, likely due to greater soil moisture and ground water availability. The soil CO_2 flux seasonal patterns were strongly driven by soil temperature, modulated by canopy structure and phenology that differed greatly between the aspen and conifer forests. Forest type differences were also observed in the radiocarbon source partitioning results, where microbial respiration was more consistent and dominant in the conifer stand (ranging between $62\text{--}70 \pm 5\%$) over the summer months. Whereas in the aspen stand, microbial respiration was more seasonally variable ($47, 73, 29 \pm 8\%$ in July, August, September, respectively) and the contribution from root respiration was greater.

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

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Wildfire significantly changes the composition and quantity of forest biomass, converting lignin and polysaccharide rich and relatively degradable carbon pools to polycyclic aromatic and charcoal rich and recalcitrant black carbon. Abundance and distribution of these carbon pools are affected by the severity of a wildfire and the intensity and frequency of post-fire rainstorms. However, there is no comprehensive knowledge available about the impacts of both fires and post-fire rainstorms on the fates of pyrogenic organic carbon (PyOC) and nitrogen (PyON) in burned terrestrial and aquatic ecosystems. To address the knowledge gap, researchers will collaborate with scientists at U.S. Forest Service and

Oak Ridge National Laboratory to conduct watershed-scale wildfire experiments in the DOE Savannah River Site, SC. Production, composition, fluxes, and temporal dynamics of PyOC and PyON in both soil and surface runoff under different severity of wildfires as well as intensity and frequency of post-fire rainstorms will be determined in the field conditions. Leachability, degradability, and mobility of PyOC and PyON will be quantified in controlled conditions. Microbial communities will also be assessed for resistance and resilience as well as function in relation to watershed perturbation and post-fire nutrient pools. Data obtained from the experiments will be used to develop, calibrate, and evaluate a reactive transport model of PyDOM and nutrients in burned landscapes. The results from field and laboratory experiments will be used to develop a reaction network accounting for dissolved and particulate BC and BN and production of carbon (C) and nitrogen (N) gases. The reaction network will be implemented in the PFLOTTRAN software. Flow and transport of particulate and dissolved phases will be modeled with ATS, which uses the Alquimia interface to access PFLOTTRAN's reaction capability. Key parameters appearing in the flow and reactive transport model will be estimated by uncertainty-aware inverse modeling using the measured C and N fluxes. ATS-PFLOTTRAN models of the plot and small watershed experiments will then be used to assess transferability of estimated parameters across scales.

How Does Mercury Methylation Respond to Intensive Forest Management and the Creation of Anoxia in Floodplain Soils?

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It is well known that silvicultural practices such as clear-cutting and thinning would alter productivity and hydrology of forest watersheds, which may also mediate a mercury (Hg) cycling response involving methylmercury (MeHg) production. In this study, researchers conducted a field study with three transects covering the upland, midland riparian, and wetlands within thinned, clearcut and uncut control areas within a first-order watershed in the lower Atlantic coastal plain on the Santee Experimental Forest in South Carolina, each transect is instrumented to monitor soil moisture, temperature, redox, water table depth, and insolation.

Commencing July 2021, researchers collected monthly composite soil samples (0–10 cm) at each site. To date, researchers found that the soil organic matter content increased significantly from upland (7.46%) and midland (9.37%) to lowland (18.55%; $p < 0.05$). Due to the intimate association of Hg with soil organic matter, total Hg content has followed this trend, i.e., upland (35.00 ng/g) and midland (48.49 ng/g), to lowland (75.14 ng/g; $p < 0.05$). Researchers also observed a similar spatial trend of toxic MeHg, i.e., upland (0.34 ng/g) and midland (0.35 ng/g), to lowland (0.50 ng/g; $p < 0.05$). When researchers compared MeHg levels across treatments at the same spatial position of the transect, researchers found that soils had much significantly higher MeHg in both harvest (0.75–0.77 ng/g) and thinning (0.66–0.70 ng/g) treatments in both upland and midland than the control upland and midland (0.34–0.37 ng/g; $p < 0.05$), but researchers found the opposite results for the lowland wetland site (i.e., 1.59 ng/g for control, 0.79 ng/g for harvest, and 1.32 ng/g for thinning). Researchers completed mercury analyses in Spring 2023. This poster will present the near final analysis of the data.

Deciphering Controls on Nutrient and Contaminant Migration Within Floodplains: The Critical Role of Redox Environments on Metal-Organic Complexes

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Whether of natural or anthropogenic origin, the fate and transport of metal nutrients and contaminants in soils and sediments is controlled by a complex network of biogeochemical reactions coupled with hydrologic processes. Dissolved organic matter (DOM) exerts a major control on metal mobility in surface and subsurface systems, albeit one that is poorly understood. Divergent OM transformation pathways drive variation in the chemical composition of DOM across watersheds. Yet, how this variation influences the functional composition and metal binding properties of DOM, along with the fate of metals and carbon, remains largely unexplored.

The overarching goal of the project is to determine the effect of redox conditions resulting from differing hydrologic regimes on formation and transport of metals and carbon. To meet the research goal, researchers used a combination of field measurements and laboratory experiments to examine the relationships between redox conditions, functionality

of dissolved organic matter, and metal speciation. Continuous monitoring of floodplain biogeochemical conditions through climatic extremes at East River, along with a newly developed analytical method, provides a unique look at metal-OM complexes. To fractionate and quantify unknown metal-organic complexes, the team developed a novel LC-ICP-MS approach, which enabled quantitation of multiple metals bound to chemically distinct fractions of DOM. Researchers also paired field experiments with multiomics (metabolomics and metatranscriptomics) techniques to examine the fate of nutrients and contaminants and compare seasonal flooding impacts in extreme low and high river discharge years, foreshadowing climate change projections. During flooded periods, microbial reduction of iron mobilized previously mineral-bound organic carbon, enhancing export of dissolved organic carbon (DOC). At the same time, flooding decreased carbon dioxide (CO₂) production and selectively preserved chemically reduced organic solutes due to metabolic constraints on microbial respiration. The onset of low-water conditions leads to re-oxygenation of floodplain soils, resulting in entrapment of DOC by newly precipitated iron minerals. Hydrologic extremes were dominated, however, by the beaver activity and the formation of a beaver dam during low water conditions, resulting in divergent water flow that yielded enhanced nitrogen removal and carbon preservation.

This work is advancing a process-based understanding of nutrient and contaminant fate and transport within watersheds, focusing principally on the dynamic hydrologic states of riparian zones. Ultimately, this work is helping to advance a robust predictive understanding of how hydrologic changes in watersheds affect water quality and element cycling, including carbon and metals.

Genome-Resolved Metagenomic Analysis of Nitrogen-Cycling Microbial Communities in Hydrologically Variable Floodplain Sediments from Riverton, Wyoming

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Despite the tremendous biogeochemical importance of nitrification, denitrification, and dissimilatory nitrate

reduction to ammonia (DNRA) in floodplain soils and sediments, remarkably little is known regarding the microbial communities responsible for mediating these processes. To address this knowledge gap, researchers have employed genome-resolved metagenomics to examine the phylogenetic diversity and metabolic potential of subsurface nitrogen (N)-cycling microbial communities within sediment cores collected from hydrologically variable floodplain sediments in the Wind River Basin near Riverton, WY. The metagenomic analysis encompasses over 70 samples collected across multiple sites, depths, and time points within the Riverton floodplain, allowing for both spatial and temporal investigations at different scales. For example, researchers have carried out a highly depth-resolved analysis of 13 depths along a 234 cm profile collected from Riverton site KB1 in 2015. At nearby site Pit2, the team collected 40 samples over both time (April to September 2017) and depth (seven distinct subsurface layers within ~170 cm cores) across a full seasonal hydrologic cycle of water table rise, flooding, and summer drought. Finally, in 2019 the team collected depth profiles (down to 180 cm) from site PTT1 in June (several days post inundation), August (peak evapotranspiration), and October (plant senescence). Along with extensive geochemical and 16S rRNA amplicon sequencing data for the wide array of 70+ samples mentioned above, researchers have generated 1000s of metagenome-assembled genomes (MAGs; 50 to 100% complete), many of which correspond to N-cycling taxa. The most in-depth work has focused on MAGs corresponding to ammonia-oxidizing archaea (AOA), which are incredibly diverse (including numerous *Nitrososphaeria* and *Nitrosopumilales* lineages) and whose community composition shifts dramatically with depth and relative to the water table. Researchers have also examined the phylogenomic diversity of nitrite-oxidizing bacteria (NOB)—capable of oxidizing the nitrite produced by AOA to nitrate in these sediments—which include diverse members of the *Nitrospinaeae* and *Nitrospiraceae*. Currently, researchers are exploring the distribution and extensive diversity of MAGs containing genes encoding one or more enzymatic steps of the denitrification or DNRA pathways (e.g., *nar/nap*, *nir*, *nor*, *nos*, *nrf*), allowing researchers to assess the potential for metabolic handoffs within both the aerobic and anaerobic N-cycling microbial communities at Riverton. Overall, this project is yielding critical genomic and ecophysiological insights into the microbial communities responsible for N-cycling in a terrestrial subsurface ecosystem directly influenced by hydrological fluctuations.

Virtual

Characterizing Deep Critical Zone Hydrologic Function in Mountainous Systems

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Researchers are working to characterize and model deep groundwater system dynamics across a gradient of landscape and sub-surface properties in montane to subalpine watersheds in west and central Montana and central Colorado. Multilevel groundwater wells were installed in a variety of landscape positions and subsurface geology across the different watersheds. Borehole geophysics, core logging and slug tests characterize subsurface structure and hydraulic properties at drilling locations. Continuous water-level and temperature logs provide information on seasonal hydraulic dynamics. Environmental tracers (i.e., chlorofluorocarbon, sulfur hexafluoride, tritium, helium-3, stable noble gas isotopes, stable isotopes of water) collected in wells and adjacent streams provide information on timing, location, and volume of groundwater circulation.

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 1000 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.

Particulate Organic Matter Transport and Transformation at the Terrestrial-Aquatic Interface

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Over the past 3 years this ESS-SBR funded research has been examining particulate organic matter (POM) dynamics in near-surface sediments of the Columbia River through coupled field and laboratory experiments. Novel, riverbed POM traps designed cooperatively with the Pacific Northwest National Laboratory field team, were deployed in the near surface riverbed within the 300 Area. The deployment of these traps was timed to capture POM infiltration into riverbed sediments during low and high flow conditions. After deployment, materials from depth sections of each of the three traps were wet sieved to obtain the fine-grained fraction (< 250 μm), which was then analyzed in triplicate for POC/PON content. The trap deployments have revealed substantial POM accumulation in the upper 20 cm of sediment. Greater accumulation occurred during elevated river flow/elevation in June/July compared to February/March. Reactive transport simulations in which fluid flow and solute/colloidal POM transport were modeled using measured hourly hydrologic gradients between river and ground water provide an explanation for these results where elevated rates of suspended POM-containing fluid flow into the riverbed lead to major POM accumulation through filtration and sorption processes. The boundary condition for suspended POM at the riverbed surface, as well as the POM filtration and sorption parameters were constrained by a combination of *in situ* measurements, POM transport experiments, and modest parameter fitting to produce estimates of POM accumulation that approximated observed levels of accumulation in the POM traps. Enhanced POM accumulation during periods of high fluid influx to the riverbed releases soluble labile DOC whose coupled transport and metabolism lead to periods of pore fluid dissolved oxygen (DO) depletion. These results provide a compelling illustration of how *in situ* (i.e., field-scale) experimentation can be coupled with modeling (i.e., the ModEx paradigm) to reveal system feedbacks and dynamics.

Resolving Flow-Dependent Indicators of Groundwater Exchange in the Columbia River, Washington

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Hydrologic exchange flows (HEFs), the movement of water between a river channel and the adjacent subsurface, are important for water quality and river corridor ecosystem function. The spatial distributions of HEFs in rivers are influenced by hydrologic conditions in the surrounding aquifer, hydraulic conditions in the channel, and the spatial distribution of alluvium with variable sediment properties under and around the channel. Exchange with adjacent aquifers is less understood in large rivers because tracer injections and other techniques one might use in streams are much more difficult due to water depth and higher flows. In this study researchers ask whether large-scale geologic units in the area drive HEF locations more than the finer-scale sediment types and the riverbed morphology along a 75 km reach of the Columbia River near the Hanford Site in eastern Washington. To determine the locations of HEFs, the team measured temperature, specific conductance, and dissolved Radon-222 along the riverbed during three sampling events in 2021/2022. The team used a FloaTEM system to identify the locations of changes in the large-scale geology and compared these to the locations of HEFs.

Together these methods provided a more complete picture of what drives HEF locations. Researchers observed water quality anomalies in similar locations to 3D numerical modeling experiments and past field research in the study area but did not find a single factor that completely explained the locations of HEFs. Though sensitive to surface water inflows, this method is useful for quickly surveying long reaches of river and determining locations for more in-depth investigations of HEF dynamics.

Student

Response of Subsurface Carbon Transformation and Transport to Changing Mountain Hydrology

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Headwater streams drain about 70% of the United States' land area and receive fluxes of terrestrial carbon matching net ecosystem production. In many parts of the U.S. Rocky Mountains, warming temperatures are responsible for reduced snowmelt inputs and waning stream discharge, leading to shifting flowpaths and subsurface biogeochemical processes that produce mobile carbon. These intertwining processes challenge the quantification and mechanistic understanding of carbon response to warming. Here, the project asks the question: how does subsurface carbon transformation and transport respond to changing hydrology in a warming climate? Researchers focused on the Coal Creek watershed in Gunnison County, CO, where temperatures have been warming 0.44°C/decade ($R^2=0.66$, $p<<0.01$). Using stream discharge and dissolved organic and inorganic carbon (DOC and DIC) data, the team calibrated a watershed-scale reactive transport model (HBV-BioRT) from October 2015 to September 2021 to understand shallow/deep flowpaths and corresponding carbon transformation and transport. Subsurface reactions were added incrementally, starting with shallow soil respiration followed by deep carbon respiration and sorption processes. This revealed shallow soil processes primarily contribute to stream DOC and DIC during snowmelt, but respiration in longer and deeper flowpaths is essential to reproduce observed DOC flushing and DIC dilution patterns. The fluxes of DOC and DIC from the shallow soil vary significantly across seasons and peak during snowmelt. Annual carbon fluxes depend mostly on the size of snowmelt. DOC and DIC production rates can increase by 50% to 70%, and export rates can increase by 70% to 90% from dry years to wet years. Conversely, carbon transformation and export from deep groundwater flow remains relatively constant across discharge regimes, but the fraction of deeper carbon export becomes much more pronounced in drier years. This work highlights the sensitivity of carbon production and export

rates to changing hydrology in mountain climate, especially snowmelt size. These shifts can have important implications for instream processes, carbon dioxide gas evasion, and carbon cycling in warming mountain catchments.

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

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Large uncertainties persist regarding forest responses to chronic climate change, especially with episodic drought disturbance. This is due, in part, to a lack of understanding of how forest composition and structure interact with physical landscape heterogeneity to influence ecosystem function and vulnerability. Tree species differences in hydraulic traits influence sensitivity of transpiration to moisture deficits, as well as sensitivity of growth, mortality, and fire risk during drought. Understanding species differences is critical for projecting future changes in forest structure and hydrological fluxes. Also, in mountainous regions, exposure to climate variability is mediated by microclimatic conditions that vary by topographic position. Forests occurring in high elevation, lower radiation, or convergent topo-positions are expected to be buffered from historical and future droughts. Alternatively, they may be more sensitive to future droughts compounded by warming due to maladapted stand structure and composition. Similarly, where stands are already exposed to high radiation and low moisture, they may be less sensitive to additional drought and warming, especially if dominated by drought-tolerant species, or, alternatively, warmer droughts could push the stand over a threshold to a nonforest state. These divergent possibilities have implications for watershed function.

The project is pursuing four hypotheses in a high-elevation, low diversity Rocky Mountain watershed:

- (1) Rooting depth and stem capacitance, more so than other hydraulic traits, explain the differences in diurnal and seasonal transpiration patterns and in growth

sensitivity to climate across the watershed's four dominant tree species.

- (2) Across forest stands, soil moisture, transpiration, canopy water content, and radial growth covary with stand density, leaf area, species dominance, and topographic position.
- (3) Interannual differences in stand-scale soil moisture, canopy water content, transpiration, and growth are smallest in convergent, high-elevation topographic positions with low incident solar radiation where the residence time of soil moisture is longest. Interannual differences are expected to be largest in convergent zones with high incident radiation, where maximum transpiration and the potential range of fluxes is very high.
- (4) Forest structure and composition have little influence on seasonal soil moisture and transpiration dynamics at landscape positions with convergent topography or where subsurface lateral flow contributions are high but have stronger influence on these dynamics in divergent and neutral positions, particularly during drought.

The approach integrates: (1) field measurements of tree hydraulic traits, transpiration, canopy water content, tree ring-width variation, and soil moisture; (2) airborne observations of transpiration and canopy water content; and (3) coupled 3D hydrologic-vegetation demographic modeling using the ParFlow-FATES-Hydro model.

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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Plant responses to water limitations involve a complex set of interactions with soil, the atmosphere, and other plants. While there is strong fundamental knowledge about the key processes through which plant hydraulics affect productivity, researchers currently lack several key components necessary for a predictive understanding of ecosystem response to future climate conditions. These components include:

(1) mechanistic understanding of plant-mediated hydraulic processes in under-studied systems, and; (2) representations of biophysical factors affecting coupled water-carbon cycles in models. To address these challenges, researchers will employ a Model-Data Experiment (ModEx) design informed by the project team's previous field experiments and numerical model development. To improve the mechanistic understanding of coupled carbon-water processes and to collect necessary data to parameterize and test models, researchers will conduct an intensive set of field measurements at existing AmeriFlux sites operated by the project team. This project will focus on longleaf pine ecosystems, once a dominant forest type in the region that is undergoing large-scale efforts to restore it through much of its native range. The work will examine plant-level hydraulic coordination of groundwater and soil water uptake, hydraulic redistribution (HR), plant water storage (PWS), transpiration, and leaf-level conductance, as well as competition among plants and the combined effects of hydrologic processes on ecosystem carbon dynamics. To address mechanisms missing in current land surface models, researchers significantly expand the functionality of an existing numerical model, developed by members of the project team, by adding components to resolve dynamic groundwater-root-hydraulic interactions and ecosystem respiration. The result will be a novel model that can resolve fully coupled interactions between groundwater, soil moisture, plants, and the atmosphere. Researchers use the extensive field measurements to parameterize and validate the expanded functionality of the new model and use it to test hypotheses that isolate the processes that compete for plant-stored water and quantify the resulting effects on ecosystem water and carbon fluxes. Finally, a series of simulations driven with E3SM future climate scenarios will predict the ability of HR and PWS to buffer longleaf pine productivity under projected extremes of the hydrologic cycle, including higher vapor pressure deficit and periods of drought. To date, in the first project year, researchers have installed a series of groundwater and soil moisture sensors provided by the AmeriFlux Management Project Year of Water project and have begun collecting new observations of tree sap flow and hydraulic conductance parameters.

Virtual, EPSCoR

Hydrodynamic Influences on the Transport of Motile Bacteria in Porous Media

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The transport of motile bacteria in porous media is relevant to many fields, but gaps remain in the understanding of the impacts of hydrodynamics and pore structure on bacterial transport. Two dimensional micromodels, designed with staggered arrays of equal diameter grains (cylinders), were used to visualize behavior of different motile species of metal-reducing bacteria under variable flow rate and porosity conditions. The team's observation and analysis of the videos of individual cell trajectories showed that at higher flow rates, motility is less important to the transport of bacteria, and that reduced motility results in reduced dispersion. Spatial variations in flow velocities (and shear) add another level of complexity to bacterial transport. Movement of bacteria from low-shear to high-shear regions located near surfaces (termed shear trapping) is generally thought to be one of the mechanisms that drives initial colonization of curved surfaces and of microfluidic pore channels. Interestingly, the team observed that the transition from a motile to a shear-dominated transport regime occurs at similar flow speeds for all species, regardless of their motility type. Furthermore, for the flow rate and porosity conditions tested, researchers did not see evidence of shear trapping causing motile bacteria to accumulate in low velocity regions in porous media. Instead, the results show that irrespective of porosity, flow rate or motility type, bacteria tend to accumulate in the medium velocity regions. This work thus aids in development of a revised picture of bacterial transport in confined porous media under dynamic flow field conditions.

Climate and Hydrological Influences on Riverine Dissolved Organic Carbon Exports in a Changing Arctic

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This project aims to advance understanding of lateral land-ocean flows of freshwater and dissolved organic carbon

(DOC) to coastal zones in Arctic regions. Hydrological cycle intensification and permafrost thaw are among a myriad of changes unfolding across Arctic regions that are impacting riverine freshwater and DOC exports. Recent progress and project results have contributed to a growing body of evidence documenting increases in exports of DOC, cold season discharge, and associated subsurface flows. Building on these efforts, researchers used meteorological data from atmospheric reanalysis and two global climate models to drive simulations with the Permafrost Water Balance Model across the pan-Arctic drainage basin over the period 1980 to 2100 to better understand likely impacts of the changes. Model simulations were validated with observations of active-layer thickness, snow sublimation, evapotranspiration, and river discharge. An acceleration in simulated river discharge over the recent past is commensurate with trends drawn from observations and reported in other studies. Increased seasonal maximum active-layer thickness in northwest Alaska during this century is congruent with simulations by the Advanced Terrestrial Simulator, which show a deepening from approximately 50 to 160 cm. Permafrost extent in the simulations declines by 42% to 63% between early (2000 to 2019) and late (2080 to 2099) century periods, while annual total runoff increases by 21% to 33%. Also consistent with other recent studies, the fraction of subsurface to total runoff increases by 29% to 44% during this century. Soil moisture tends to decline, despite the runoff increases, influenced by higher evapotranspiration rates and drainage through more thawed soils. These manifestations of hydrological cycle intensification and permafrost thaw have profound implications for Arctic-terrestrial and coastal environments influenced by river flows and the materials they convey.

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

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Plants passively move water around in the subsurface from wet to dry soil via their roots in a process known as hydraulic redistribution. Soil moisture is an important regulator of microbial activity, organic matter decomposition, biogeochemical cycling, and soil properties. This passive redistribution of soil water may have important implications for a soil's carbon carrying capacity, nutrient exchange, and soil structure, particularly in water-limited environments such as the

Mediterranean climate of the Western U.S. The project seeks to elucidate the relationship between hydraulic redistribution, soil nutrient dynamics, and soil properties through a multi-year study, which will combine data from a controlled greenhouse experiment with *in situ* data collected from two adjacent hillslopes at the H.J. Andrews Experimental Forest; one which is known to experience hydraulic redistribution, and one which experiences little to no hydraulic redistribution. Recent work has revealed two types of ecohydrologic function associated with high and low hydraulic redistribution among the hillslopes of the Andrews Forest. Where trees have access to groundwater, moisture in the upper soil profile increased by nearly 2% daily. In contrast to this, hillslopes where tree access to groundwater is inhibited experience a daily moisture increase in the upper soil of < 0.5%. Both types of ecohydrologic function have been documented on two adjacent hillslopes in the Andrews Forest. The study will build on existing techniques for the identification and quantification of hydraulically redistributed water by combining transpiration and physiological measurements of trees with new geophysical methods for mapping the magnitude, location, geometry, and flow paths of near surface water. In conjunction with these techniques, researchers will be quantifying soil carbon pools via data collection of soil respiration and soil-carbon chemistry analyses. Furthermore, the classification of soil physical and hydrologic properties will be done through field and laboratory methods. Combined, this data will help us 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.

Student

An Ecophysiological Perspective of Hydraulic Redistribution: Feedbacks on Soil, Fungal, and Root Morphologies

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Hydraulic redistribution is the passive movement of water within the soil profile from wetter areas to drier areas via biological pathways such as roots and fungal hyphae. Hydraulic redistribution of soil water into the upper soil horizons may have important implications on root morphology and soil biota, particularly in water-limited environments such

as those of the western United States. The reduced rates of soil drying through periods of drought, which results from the passive regulation of near-surface soil water, may limit fine root desiccation, reduce root embolism, increase the lifespan of roots, enhance overall rooting architecture, and help to maintain important mycorrhizal interactions. This project will explore the dynamic relationship between the rooting, fungal, and soil morphologies under Douglas-fir (*Pseudotsuga menziesii*) across different water availability regimes and seek to understand how these morphologies influence the magnitude, timing, and flow paths of water redistribution to near-surface soils. To achieve this, the team will combine a multiyear greenhouse experiment with a field study at H. J. Andrews Experimental Forest on two adjacent hillslopes, which have been shown to exhibit two contrasting hydraulic redistribution regimes as demonstrated through previous study of the site. Using microcomputed tomography of soil cores, researchers will be able to characterize the spatial distribution of soil pores and derive a detailed understanding of soil morphological characteristics. This will be combined with reconstruction of rooting architecture in the greenhouse experiment through destructive sampling of pots throughout the course of the experiment and in the field through existing methods of characterizing root abundances in soils. Furthermore, the quantification of fungal and mycorrhizal concentrations throughout the rooting profile will be obtained through hyphal-length analysis. The identification and quantification of hydraulically redistributed water will be measured by building on existing methods of sap-flow and water content measurements, with the deployment of new geophysical techniques for the detailed mapping of the magnitude and flow paths of near-surface water. Taken together, these data will help to clarify the complex feedbacks between subsurface hydrology, rooting and fungal behavior, and soil morphological properties.

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

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In mountainous watersheds, rivers typically have an armor layer of coarse sediment that protects the finer subsurface from erosion. In theory, armor layer motion during high magnitude flows could release the subsurface fine sediments that are often enriched in phosphorus and particulate organic carbon (POC). Hysteresis in POC, soluble reactive

phosphorus (SRP), particulate phosphorus (PP), total phosphorus (TP), and suspended sediment (SS) may therefore be partly controlled by armor layer motion. In addition, streambed concentrations of these constituents may depend on whether a reach is losing or gaining. The project tests whether armor layer motion and streambed concentrations influence hysteresis patterns during summer monsoon flows in one gaining and one losing reach of La Jara Creek in Valles Caldera National Preserve, NM. Researchers measure the amount and timing of armor layer motion, streambed and river concentrations of POC, PP, SRP, TP, and fine sediment, as well as surface flow and groundwater exchange in these two reaches. In addition, the team conducted artificial floods that isolated the effects of armor layer removal on nutrient and fine sediment concentrations in the water column. Hysteresis in SS, TP, and PP occurred during these artificial floods, demonstrating the ability of the armor layer to control hysteresis because all other potential sources of these constituents were eliminated. Equilibrium experiments suggested that streambed sediments are a potential source of SRP to the water column, which was observed in natural flow events. Preliminary results also demonstrate that SS, turbidity, PP, TP, and POC often follow the same hysteresis pattern in a given natural flow event, implying that they may have a similar source. Hysteresis of these constituents changes between clockwise and counterclockwise in different natural flow events and may be related to the amount or timing of armor layer breakup or the streambed concentrations, which the team is currently investigating. The final results of this work will determine how perturbations, such as the sequence and magnitude of droughts and floods, constrain biogeochemical nutrient cycling and impact subsequent temporal variations in nutrient and fine sediment export from mountainous watersheds.

Watershed Controls on Uranium Concentrations Tied into Natural Organic Matter and Iron Interactions in Streambeds and Wetlands

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Wetlands and hyporheic zones are critical interfacial regions with complex and seasonally varied dynamics in hydraulic, chemical, physical and microbial properties. Different environmental conditions result in their functioning as a sink or source of organic matter (OM) and associated contaminants, such as uranium (U). In this project, researchers

tested the central hypothesis that watershed interfacial zones, including wetlands and hyporheic zones, produce unique yet characterizable OM especially at gaining sites, where OM- and iron (Fe)-rich flocs form. The mixing models of Tims Branch combined with stable isotopes of ²H and ¹⁸O corroborate sources and sinks of the subsurface and surface waters along the flow path (Santschi et al. 2023). Sixteen sediment samples were collected from gaining and losing sections of Tims Branch to allow evaluation of the compositional differences of their sediment organic matter (SOM). The SOM samples were extracted from the sediment through the use of an optimized method (Xu et al. 2023a) with techniques including solvent extraction, ultrafiltration, and solid-phase extraction. Results showed the following SOM characteristics: (1) the average molecular weight of SOM in gaining site is lower than that in losing site; (2) sulfur to carbon ratio are higher in gaining site; (3) SOM is more oxygenated in gaining site; (4) nominal oxidation state of carbon (NOSC) is higher in gaining than losing; (5) the dominant compounds in losing site are protein, lignin, and lipid whereas in gaining site they are lipid, fatty acids, and condensed aromatics; (6) there are more aromatic or condensed aromatic in gaining than losing site; (7) there are more U-containing organic compounds in gaining site, especially in the low- molecular-weight fraction (< 3 kDa). Moreover, their moieties are spread over the van Krevelen diagram suggesting a possible unspecified compound class with a unique functional group responsible for U binding in these two regions. Microbial analysis (16s rRNA) concurrently supports that a unique microbial community evolves in a floc sample from a gaining site that participates in the modification of the SOM. The orange-colored NOM- and Fe-rich floc hotspots in the gaining stream showed a unique composition with abundant CONPS signatures in their ESI-FT-ICR-MS spectra, as well as in microbial community composition and genetic make-up, where Fe-driven redox and microbial processes can mutually control NOM functionalities, and vice versa, leading to flocs acting as terrestrial OM traps (Xu et al. 2023b).

Multisystem Feedbacks from a Changing Climate: Do Altered Hydrological Dynamics Control Vadose Zone Carbon Nutrient Cycling and Storage in Shallow Aquifer Systems?

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The vadose zone, which extends from upper soils to the subsurface water table, consists of many distinct habitats (including the critical zone), each with its own physical characteristics. Upper soils are typically richer in organic carbon, chemical diversity, and concentration, while deeper portions near the water table have less labile carbon and a greater percentage of humic acids and other long-lived organics. The availability of carbon and oxygen constrains the habitability of these zones. Typically, microorganisms (bacteria, archaea, and fungi) extend throughout the vadose zone and potentially deeper into the bedrock, while higher eukaryotes (i.e., arthropods and plants) are limited to the surficial soils. An exception to this is deep taproots of some tree species that can extend tens of meters into the subsurface. In subsurface systems, microbial metabolisms are constrained by the availability of carbon (organic and inorganic) and electron acceptors. In snow-dominated forest systems, water recharge of shallow aquifers is often driven by snowmelt rather than rainfall. Thus, the flux of dissolved carbon and other nutrients, like nitrogen and phosphorus, from upper soils to the deeper vadose zones occurs primarily during the spring thaw. As water recharges the system, gradients of oxygen and the presence of alternative electron acceptors will dictate which microbial metabolisms may operate and whether methane is consumed or produced. In other shallow systems, simple organics like acetate can elicit a sweeping microbial response that can drive fermentation and methanogenesis deeper into the vadose zone and heterotrophic respiration with oxygen in shallow portions. Thus, the role of water, and its ability to limit oxygen diffusion, will have immense regulation over microbial metabolic activity and, by extension, the classes and amounts of carbon that persist. As regional climates change due to warming, northern Minnesota is experiencing extended growing seasons, higher evapotranspiration, and altered precipitation patterns. The project's main questions revolve around how disruptions in water delivery to subsurface systems coupled with enhanced water usage from the forest community will affect subsurface cycling and ultimately the emission

of key climate-impacting compounds like carbon dioxide, methane, and nitrous oxides.

Early Career

Enhanced Chemical Weathering from Geomorphic Features in the East River Watershed, Colorado

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Physical and chemical weathering in Earth's high-elevation regions provides sediment to downstream fluvial systems, controls river chemistry, and regulates long-term climate. Mountain landscapes contain a diverse set of landforms generated by geomorphic processes, including landslides, moraines, and rock glaciers. These landforms generate unique flowpaths and water-rock interactions for precipitation as it moves through the critical zone before becoming streamflow.

Prior work has identified landslide deposits as “hotspots” that increase dissolved solute concentrations in tectonically active mountains, but there is still considerable uncertainty as to the magnitude of which geomorphic processes influence solute chemistry across different tectonic and climatic regimes. The team measured cation and anion concentrations in 79 surface water samples collected from areas that drain a variety of geomorphic features in the East River watershed in Colorado. The results show that landslides produce higher solute loads than streams draining soil-mantled hillslopes long after landslide occurrence. Watersheds with evidence of active bedrock incision also generate high solute concentrations, whereas solute concentrations in surface waters draining glacial moraines and rock glaciers are comparable to values from watersheds draining soil-mantled hillslopes. The results have implications for understanding the sources of solute generation in alpine watersheds, including hotspots for chemical weathering and temporal variability in weathering rates.

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

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

important for correctly predicting the magnitude of hyporheic biogeochemical transformations, with important implications for material processing in watersheds.

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, 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 were combined with metaomic signals of the active microbial populations in riparian and hyporheic sediments of Steed Pond at Savannah River National Laboratory to predict the role of hydrological forcing on the spatiotemporal transformation of carbon, nutrients, redox processes, and GHG emissions along this gaining and losing wetland stream. Two *in situ* electrochemical systems and a suite of monitoring wells were deployed at two locations along Steed Pond to monitor the temporal variations in pore water redox biogeochemistry at four different depths and relate these changes to the local hydrology. Simultaneously, sediment samples were collected at each site under different hydrological conditions to extract DNA, RNA, and proteins for *in situ* multiomic analyses that will shed light on the microbial metabolic processes affected by hydrological changes. In parallel, homogenization models were developed to calculate the stiffness and diffusivity tensors of porous media with thin ellipsoidal flow paths and small spherical voids.

Upscaling was extended to permeability to predict the effect of reactive flow on the microstructure and physical properties of sediments subjected to hydraulic forcing. Reactive flow was then simulated in one dimension with the open-source finite element software PFLOTRAN for simplified problems. PFLOTRAN will be used to validate the homogenization models and solve large-scale boundary value problems by assigning a homogenized constitutive law with spatially variable parameters sampled from the field to the sediment. 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 carbon 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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Wetlands are terrestrial-aquatic interfaces that serve as biogeochemical control points regulating the removal of anthropogenic nitrogen (N) 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 quantity and composition of OM can affect whether N is removed or recycled via competing microbial pathways, therefore, researchers hypothesized that flood disturbances will heighten the differences in nitrate reduction pathways by delivering soil-derived OM to hillslope wetlands and stream-derived OM to floodplain wetlands. Researchers conducted a study investigating how hydrologic connectivity mediates wetland biogeochemical response to floods at a forested, headwater coastal plain system where elevational differences have resulted in wetlands along a gradient of hydrologic connectivity, ranging from shallow subsurface flowpaths in the hillslope and surface inundation in the floodplain. Researchers designed the project to adhere to

ICON science principles that is, to Integrate work across disciplines and scales; Coordinate use of consistent protocols; support Open exchange of ideas, and to use a Networked approach to data generation through stakeholder engagement. Researchers installed piezometers in nine wetlands along a gradient of hydrologic connectivity to characterize wetland hydrology during flood events. Researchers measured nitrogen removal (denitrification, anammox) and recycling (dissimilatory nitrate reduction to ammonium; DNRA) potentials in wetland soils along the hydrologic gradient using isotope pairing on soil slurries. Researchers also measured dissolved inorganic nitrate-nitrite in surface water and percent OM in soil (loss on ignition). Researchers found that during the dry season (baseflow), hillslope-connected wetlands had a lower OM: nitrate ratio that likely promoted denitrification over DNRA, as denitrification rates were nearly twice as high in hillslope-connected wetlands compared to floodplain-connected wetlands. In contrast, DNRA dominated in floodplain-connected wetlands and rates were nearly double that of hillslope-connected wetlands. Future event-based sampling efforts will relate changes in flood-derived organic matter composition to nitrate reduction rates following flood disturbances. In the second year of the study, these data will be paired with event-based wetland- and watershed-scale N measurements to develop a hydro-biogeochemical model to assess how post-flood N processing impacts watershed N impact.

Applying “R-Osmos” to Quantify Hot Moments in a High Mountain Watershed: Co-Development of Novel Methodology to Advance Terrestrial–Aquatic Interface Models

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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 (CH₄) oxidation and nitrate reduction at DOE's East River Watershed Function science focus area (SFA). Researchers will deploy novel, continuous, time-integrating, *in situ* microbial rate samplers to inform

the magnitude and variation in biogeochemical processes across the terrestrial–aquatic interface, which, upon completion, will be used to refine a reactive transport model for this area. To accomplish this goal, the team will use uniquely configured osmotic samplers (OsmoSamplers) to continuously quantify the rate at which microbial communities transform methane and nitrate on either side of a meander. OsmoSamplers use a diffusion gradient to slowly pump water into tubes of such small diameter that sample mixing is negated. Multiple OsmoSamplers can be used together to continuously add solutes and preservatives or collect samples for later analysis, providing a record of hot moments in long-term datasets. In this work, researchers will use rate-osmotic samplers (R-osmos) to acquire spatially explicit rate measurements by adding nitrate and methane separately to discern transformation of these critical compounds. Rates will be coupled with quantifications of natural solute composition (both nitrate and CH₄) and quantitative gene abundance for the relevant processes (i.e., genes responsible for nitrate reductase and methane monooxygenase), allowing researchers to connect solute, rate, and microbiome characteristics. During its first year, the project has focused on “bench testing” the R-osmo device in preparation for a planned year-long field deployment that will commence in summer 2023. Through this, the team uncovered small, yet critical modifications to the design, making the instruments ready for deployment. This presentation will cover the overall aims of the project, update progress to date, and highlight opportunities that this research framework may provide for collaboration with other SFA users.

Leptothrix ochracea Genomes Reveal Potential for Mixotrophic Growth by Oxidation of Iron and Organic Carbon

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Iron oxyhydroxides are extremely reactive components of environmental systems, exerting a strong influence on biogeochemical cycles, so the project aims to understand the controls on iron oxidation, particularly by microorganisms. At the Savannah River Site (SRS) in South Carolina, extensive iron-oxidizing microbial mats carpet streams and wetlands, sorbing uranium and other metals, and thus mediate the transport and availability of toxins. To understand the drivers of these processes, researchers need to determine the niche and physiology of iron-oxidizing bacteria (FeOB). Neutrophilic FeOB are typically considered

chemolithoautotrophs, using the energy of iron oxidation to fix carbon, but this potentially limits FeOB impacts given the low energetic yield of iron oxidation and the high costs of autotrophy. Therefore, the team posited that wetland FeOB may in fact utilize organic carbon, making organic carbon availability an important factor in iron oxidation and metal sequestration.

The iron microbial mats in Tims Branch stream and wetlands at the SRS are comprised of iron-mineralized sheaths typical of *Leptothrix ochracea*, an organism first described in 1888 by Winogradsky, who hypothesized that it grows a chemolithoautotrophic iron oxidizer. However, it has never been isolated and does not have a complete genome sequence available, so its physiological roles in iron and carbon cycling are very limited. These iron microbial mats were analyzed using 16S rRNA molecular surveys and by SILVA classification. *Leptothrix* was poorly detected (up to 0.004%) despite the obvious presence of sheaths. This is consistent with the rarity of *L. ochracea* in similar molecular surveys. Researchers performed whole-genome sequencing on nine iron microbial mats from stream and wetland sites from the SRS; eight high-quality genomes of *L. ochracea* were reconstructed from these mats. A full 16S rRNA sequence was recovered from one *L. ochracea* genome, which can be used as a reference for detecting *L. ochracea*. On reexamination of the 16S data, *L. ochracea* was present up to 8.2% relative abundance. All eight genomes contained genes for iron oxidation, carbon fixation, and utilization of organic acids and polysaccharides, demonstrating the potential for *L. ochracea* to grow as a mixotroph, i.e., using both iron(II) and organic carbon. To further investigate this potential, researchers computed stoichiometric metabolic models, which demonstrated the potential for growth using lactate. In sum, results suggest that organic carbon availability is an important driver of microbial iron oxidation and associated toxic metal bioremediation in these wetland environments.

Virtual

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

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Forest disturbances are increasing globally due to the anthropogenic impact on land use and climate. For a rocky

mountain watershed impacted by bark beetle kills and wildfire, this research investigates groundwater-supported vegetation refugia as a mechanism of forest recovery at local to landscape (i.e., disturbance) scales. In the project's study area, two priority forest sites have been identified where active post-disturbance regeneration was observed, each representing an endmember in climate, dominant tree species, topography, and disturbance type/severity. The headwater site (Glacier Lakes Ecosystem Experiments Site) is an Engelmann spruce (*Picea engelmannii*)–subalpine fir (*Abies lasiocarpa*) forest recovering from a spruce beetle epidemic from 2008 to 2010. For this site, researchers have developed an integrated ecohydrological model of plant hydraulics coupled to surface/subsurface hydrology (ParFlow-TREES) to investigate the mechanisms of forest water and carbon flux recovery using 20 years of site historical eddy covariance flux data as constraints. Results suggest that during wet years, high soil moisture supported by a shallow water table resulted in enhanced spruce and fir evapotranspiration (ET) and gross primary productivity (GPP). However, during dry periods with a deep water table, tree recovery

was slowed down significantly. While this is consistent with the regeneration observations at the site since the spruce beetle disturbance, the model has also identified the important role of understory growth in facilitating forest recovery. The second site lies at the opposite end of the topography at Chimney Park, where a 2008 to 2010 bark beetle epidemic of lodgepole pine (*Pinus contorta*) was followed by the 2018 Badger Creek wildfire. For this site, the team is developing a preliminary model as well. In the coming summer field season, researchers will collect joint climate, vegetation, soil moisture, and groundwater data at both priority sites and incorporate an understory regeneration module into ParFlow-TREES as well. With the updated model, the team will simulate 20 years of ET, GPP, and soil volumetric water content and water table position at the two sites, with and without the new recovery module and with and without lateral flow. Model results will then be compared against both historical and newly collected field measurements to evaluate the importance of hydrology as well as understory in driving forest flux recovery after disturbance(s).

Science Focus Areas

Plutonium Transport in Vadose Zone Sediments Under Acidic Solution Conditions at the Hanford Site, United States

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

Between 1955 to 1962 over 4 million liters of acidic processing waste, containing an estimated 40–150 kg of plutonium (Pu), were released into the sediments of the 216-Z-9 (Z-9) trench at the Hanford Site in southeastern WA. The waste was characterized as having a high ionic strength (~5 M nitrate), low pH (~pH 2.5), and contained organic processing solvents including tributyl phosphate (TBP). The majority of the Pu precipitated in the first several centimeters beneath the unlined trench, but a small fraction was detected in the vadose zone at depths up to 37 m (Cantrell and Riley 2008). Previous research has shown that the Pu and TBP are detected concurrently in the subsurface in the sediments with the lowest pH 1; however, the mechanisms controlling past and future Pu mobility beneath the trench are unknown.

In an effort to better understand Pu migration below the Z-9 trench, scientists 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. Two types of experiments were designed to investigate (1) Pu mobility in low pH aqueous fluids and (2) Pu mobility with mixed aqueous organic fluids. The effluent was analyzed for Pu, changes in pH, and solution chemistry, and the data was compared and modeled. Results show that Pu does not become mobile until the pH of the sediments is reduced below pH 4. In low pH aqueous fluids, significant Pu mobility (14% total Pu breakthrough) is not observed until pH < 2. Pu in organic TBP-containing solvents is highly mobile in sediments that have been treated with high nitrate low pH acidic fluids. Pu can travel with these organic solvents virtually uninhibited with 94.8% and 86.8% total Pu breakthrough, observed at pH 1 and pH 3 respectively. The 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.

Cantrell, K. J., and R. G. Riley. 2008. *A Review of Subsurface Behavior of Plutonium and Americium at the 200-PW-1/3/6 Operable Units*, PNNL-SA-58953. Pacific Northwest National Laboratory. https://www.pnnl.gov/main/publications/external/technical_reports/PNNL-SA-58953.pdf

A Chemistry-Informed Hybrid Machine-Learning Approach to Predict Metal Sorption to Mineral Surfaces

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The Lawrence Livermore National Laboratory (LLNL) Surface Complexation/Ion Exchange (L-SCIE) database is a recent effort to unify community adsorption experiments and metadata in a findable, accessible, interoperable, and reusable (FAIR) format (Wilkinson et al. 2016). To date, it has mined over 27,000 raw adsorption data from the literature and provides a platform to test novel approaches to surface complexation modeling and surface complexation database development. Briefly, L-SCIE mines sorption data (e.g., K_d, % sorbed, surface excess) and dataset experimental conditions (e.g., background electrolyte, mineral surface area, gas composition) from journal manuscripts and loads them into a database. The sorption data undergo a series of unit conversions to yield a unified database that includes propagated conversion errors from the original extracted data. The database can then be filtered for a mineral-metal pair of interest to display a corresponding experimental dataset. The application of the L-SCIE database to traditional surface complexation modeling was illustrated in a recent publication (Zavarin et al. 2022).

An alternative hybrid machine-learning (ML) approach will be presented that shows promise in achieving equivalent high-quality predictions compared to traditional surface complexation models. At its core, the hybrid random forest (RF) ML approach is motivated by the proliferation of incongruent surface complexation models (SCMs) in the literature that limit their applicability in reactive transport models. This project's hybrid ML approach implements PHREEQC-based aqueous speciation calculations; values from these simulations are automatically used as input features for an RF algorithm to quantify adsorption and avoid SCM modeling constraints entirely. Named the LLNL Speciation Updated Random Forest (L-SURF) model, this hybrid approach is shown to have applicability to uranium(VI) sorption cases driven by both ion-exchange and

surface complexation, as is shown for quartz and montmorillonite cases. The approach can be applied to reactive transport modeling and may provide an alternative to the costly development of self-consistent SCM reaction databases.

Wilkinson, M., et al. 2016. "The FAIR Guiding Principles for Scientific Data Management and Stewardship," *Scientific Data* 3, 160018. DOI:10.1038/sdata.2016.18.

Zavarin, M., et al. 2022. "Community Data Mining Approach for Surface Complexation Database Development," *Environmental Science & Technology* 56(4), 2827–2838. DOI:10.1021/acs.est.1c07109.

Effects of Seasonal Anoxia on Trace-Level Natural and Anthropogenic Element Cycling in a Monomictic Pond

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This study investigated the influence of seasonal anoxia in a warm monomictic pond on the composition of the microbial community and the cycling of natural and anthropogenic elements. Pond B at the Savannah River Site (Aiken, SC) received cooling water from the R-reactor that resulted in contamination of anthropogenic radionuclides plutonium-239 and cesium-137, which can be used as tracers to monitor natural hydro-biogeochemical processes. Seasonal stratification leads to seasonally anaerobic hypolimnion and profound changes in geochemical conditions that can impact the cycling of trace elements and organic matter through the system.

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 1–2 orders of magnitude within the anaerobic hypolimnion. Plutonium (Pu) 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 iron(III)-POM (particulate organic matter). This finding is consistent with depth discrete sediment analyses, which demonstrated elevated concentrations of Pu in sediments with high organic matter. Thus, organic matter cycling likely plays a role in retaining Pu and other trace elements within the pond by causing seasonal redistribution between sediment and

overlying pond water and deposition in organic rich sediments accumulating near the outlet. Conversely, cesium concentrations were highest in the pond inlet and appear to be controlled by particulate input from the influent canal, dominated by clay, silt, and sand minerals bearing iron (Fe).

Characterization of the microbial community provided additional insights regarding the observed cycling of Fe, Pu, and organic carbon. The microbial community varied with seasonal thermal stratification with Fe(III) reducers (e.g., *Geothrix* and *Geobacter*) dominating the deep, anoxic zone and sulfate reducers and methanogens present in the anoxic layer, with all likely contributing to Fe and Pu cycling. Microbiome analyses revealed potential for three impacts on the Pu and Fe biogeochemical cycles: (1) Pu bioaccumulation throughout the water column; (2) Pu-Fe-OM-aggregate formation by Fe(II) oxidizers under microaerophilic and aerobic conditions; and (3) Pu-Fe-OM-aggregate or sediment reductive dissolution in the deep, anoxic waters. Additionally, microcosm experiments revealed that the bio-sorption capacity of plutonium to washed bacterial and algal cells (loosely bound exudates removed) is similar.

SLAC Floodplain Hydro-Biogeochemistry Science Focus Area: Soil-Gravel Bed Interfaces as a Hydro-Biogeochemical Control Point in a Mountainous Floodplain Aquifer

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Montane alluvial floodplains represent important water quantity and quality moderating ecosystems. They are characterized by heterogeneous geological architectures resulting from depositional processes. Typically, sharp (<50 cm wide) redox interfaces develop in the vicinity of lithological transitions and are associated with intense contaminant and nutrient cycling. The cumulative exchanges of water and solutes across these interfaces are challenging to assess as the direction and intensity of interfacial exchanges respond strongly to seasonal shifts in hydrology, including extreme events like flooding and drought. As climate change reshapes temperature and precipitation regimes throughout mountainous watersheds, the incorporation of hydro-biogeochemical interfaces into models could be key to predict water quality and availability in these environments.

The SLAC Floodplain Hydro-Biogeochemistry SFA developed numerical simulations of an alluvial aquifer located near Crested Butte, CO. This aquifer, which underlies the Slate River, is characterized by an extensive (3600 m²) interface between an overlying fine-grained, predominantly anoxic soil and an underlying, mostly oxic cobble and gravel alluvium. Simulation results emphasized the strong spatiotemporal variability of exchanges at the soil and gravel bed interface, which in turn determines the biogeochemical function of the soil as a potential sink or source for redox-sensitive solutes. In particular, flooding events from the construction of a beaver dam greatly increased downward drainage from the soil and the export of reduced solutes to the gravel bed, which were then quickly transported in the down-valley direction. In contrast, drought events induced upward water movement with the gravel bed acting as a reservoir for the floodplain vegetation. Thus, alternating hydrological forcings resulted in the development of a geochemically dynamic mixing zone at the interface between the gravel bed and the soil. Sensitivity analyses highlighted that the extent of this mixing zone—and more generally of the response of similar floodplain environments to hydrological shifts—is primarily linked to the geological architecture of the aquifer, with contiguous floodplain sediment layers acting as preferential flow-paths that propagate the influence of hydrological perturbations throughout the alluvial aquifer.

SLAC Floodplain Hydro-Biogeochemistry Science Focus Area: Genome-Based Analysis of Microbial Genetic Potential to Drive Shifts in Subsurface Geochemistry in Floodplain Sediments

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The Slate River (SR) floodplain experiences seasonal rise and fall in the water table related to snowmelt-induced flooding, precipitation, and evapotranspiration. These fluctuations in the water table determine the inputs of nutrients and other substances to the subsurface and oxygen penetration depth, thus strongly influencing microbial communities and biogeochemical cycling. This work has used amplicon sequencing to investigate microbial community composition across multiple depths and time points from 2018 to 2021 at two SR floodplain sampling locations (OBJ1 and

OBJ2). These spatiotemporal analyses have revealed diverse populations of bacteria and archaea—including methanogens, methanotrophs, sulfur-oxidizing and sulfur-reducing taxa, ammonia-oxidizing archaea (AOA), and iron-cycling bacteria—with striking distributions across oxic-anoxic boundaries. Further examination of the genetic potential at different depths and oxygen conditions was conducted on metagenome-assembled genomes (MAGs) from June 2018 samples from both sampling locations at depths ranging from 50–150 cm below ground surface.

The research team recovered 1233 MAGs (>50% complete) spanning 38 bacterial and archaeal phyla. Of note, many genomes were recovered for putative methane-cycling organisms. While methanogens (*Methanomassiliicocales*, *Methanoregulaceae*, *Methanotrichaceae*) are limited to deeper anoxic depths, diverse and abundant genomes were recovered from putative methanotrophs across the entire depth profile, including *Methanoperedens*, *Methylomirabilis*, and Bin18 and *Binataceae* (*Binatota*). *Methanoperedens* can have significant metabolic flexibility, coupling anaerobic methane oxidation to myriad electron acceptors (e.g., nitrate, iron, manganese, and potentially selenate, arsenate, and elemental sulfur) and can display a pleomorphic lifestyle that could allow this group to thrive in a dynamic floodplain. Other putative methanotrophs, *Methylomirabilis* and *Binatota*, occur in shallower, unsaturated depths. *Methylomirabilis* are also known for their ability to oxidize methane using nitrite (n-DAMO) and co-occur with nitrifiers in samples. In oxic depths, genomes were recovered for distinct guilds of nitrifiers, including AOA and putative comammox bacteria within *Nitrospiraceae*. Careful investigation of the recovered genomes will further elucidate connections between methane and other biogeochemical cycles. Thus far, >3700 MAGs have also been generated from samples collected in 2019 and 2020, allowing for comparison of metabolic potential before and after construction of a beaver dam near OBJ2.

SLAC Floodplain Hydro-Biogeochemistry Science Focus Area: Mechanisms Controlling Colloid Formation and Impact on Water Quality in Alluvial Sediments

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Recurring seasonal wetting and drying of soils and sediments drives redox processes at solid–water interfaces,

promoting shifts in aqueous phase parameters (e.g., pH, ionic strength, and ionic composition) and chemical, organic, and mineral transformation of the solid phase, which could generate colloids (1 nm to 1 μ m), and/or influence colloidal stability. Because they are 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 as well as the products exported to the ground- and surface waters. As an example, aqueous metal sulfide clusters, generated in sulfidic conditions, are remarkably resistant to oxidation and have been found to contribute to contaminant transport in rivers. Despite evidence that redox cycles play a significant role in generation and transport of colloids, the mechanisms and the nature and reactivity of generated colloids are poorly understood.

To resolve this knowledge gap, the research team is developing an approach consisting of detecting different particle distribution in size, chemical composition, molecular weight, and zeta potential using asymmetric field flow fractionation combined with inductively coupled plasma mass spectrometry, UV-, fluorescence-, multi-angle light scattering-, and zetasizer-dynamic light scattering detectors. The different particle distributions are thus separated and collected in redox-preserved conditions for deeper molecular-scale characterization (e.g., single particle inductively coupled plasma time of flight mass spectrometry; transmission electron microscopy; scanning transmission X-ray microscopy; X-ray absorption spectroscopy; nanoscale secondary ion mass spectrometry; Mössbauer). The research team has examined the influence of redox changes on the generation and transport of colloids through a transect from bedrock to floodplains. To date, bedrock shale oxidation lab-simulation investigations have revealed that oxidative dissolution of pyrite at neutral pH generates 50–100 nm iron (Fe) colloids, promoting the mobilization of nutrients and contaminants (e.g., nickel and chromium) through pore and fracture networks.

The team further examined the influence of sulfidation on formation of Fe colloids in floodplains, combining results from lab-simulation sulfidation of ferrihydrite aggregates and natural colloidal fraction from a redox active floodplain at Slate River, CO. While low sulfidation increased colloidal stability of ferrihydrite, higher sulfidation (sulfur/Fe < 0.5) generated nanoscale Fe(II) sulfide colloids, stabilized by oxidative impurities. However, in natural samples, ferrihydrite nanoparticles persisted under sulfidic conditions, which were attributed to the passivation by silicon and organic matter. These results contribute knowledge needed to predict redox-generated colloid-facilitated nutrient and contaminant transport in response to disturbances, such as weather events and management strategies.

Student

Observations of Hot Moments of Beaver-Driven Biogeochemical Activity in a Mountainous Floodplain Using *In Situ* Sensors

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In many mountainous watersheds, warming temperatures and declining snowpack have led to reduced river flow through the late summer and early fall, decreasing the volume of water available for agriculture, energy, recreation, and human consumption. However, in many regions, warming temperatures also coincide with an expansion in populations of the North American beaver (*Cercis canadensis*). As ecosystem engineers, beavers build dams that increase seasonal floodplain storage and that may support late-season, ground-water-fed baseflow. These hydrologic changes can also alter biogeochemical cycles within the floodplain, impacting floodplain greenhouse gas release and the export of nutrients and contaminants to surface water. In particular, sudden pulses of biogeochemical activity associated with beaver dam construction (or failure) remain poorly characterized, largely because these transient events are difficult to observe via manual sampling.

To address this gap, researchers instrumented a beaver-impacted floodplain along the Slate River, CO, with an array of *in situ* sensors monitoring water content, dissolved oxygen concentrations and carbon dioxide concentrations within fine-grained sediments. Construction of a new beaver dam in 2018 inundated portions of the floodplain and coincided with the onset of anoxic conditions in the floodplain sediments. Then, in 2021, migration of the river channel cut off the beaver dam from the main river, causing a large (20 m x 50 m) pond behind the dam to drain and allowing oxygen incursion into previously anoxic sediments. The large pond then refilled in less than 2 hours during a fall rainstorm, returning the floodplain sediments to anoxia once again. With the frequent cycling between oxic and anoxic conditions, these transient events induce pulses of biogeochemical activity that impact water quality in the adjacent river, further highlighting beavers' impact on ecosystem function.

The Influence of Wildfires on Hydro-Biogeochemical Processes: A ModEx Perspective

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

The iterative ModEx approach underpins hypothesis-driven research that advances predictive understanding of complex environmental systems. Such an approach often consists of one technical ModEx cycle that includes using experimental or field data to parameterize and calibrate models and using models to guide data collection in the field and/or in the lab. This study further defines a knowledge cycle that builds upon both modeling and experiments to generate new hypotheses that advance the state of predictive understanding.

Successful ModEx practices rely on coordinated team efforts to enable information exchange at both the technical and knowledge levels. This project utilizes this approach to understand the influence of wildfires on river corridor hydro-biogeochemistry. The Wenas Creek watershed within the Yakima River Basin was selected as a testbed, with 76,000 acres of semi-arid shrub-steppe landscape burned at low to moderate severities during the 2020 Evans Canyon Fire. Because fires directly alter landcover and surface soil properties, the research team hypothesized that wildfires would increase surface runoff and reduce infiltration, thus leading to higher and earlier peak flow in responding to precipitation events. The team used the integrated watershed model Advanced Terrestrial Simulator to study post-fire watershed hydrologic responses by explicitly representing changes in surface soil permeability and vegetation properties. By comparing simulated responses with and without fire impacts, researchers found no significant differences in hydrology. Field observations showed no statistical differences in the concentration of measured dissolved organic carbon (DOC), total dissolved nitrogen, pH, dissolved oxygen, or total suspended solids between burned and reference sites across monthly sampling for the first 2 years following the fire.

These observations fueled a new hypothesis that stream responses to fires are dependent on the relationship among

fire size, severity, and catchment characteristic. Soil and Water Assessment Tool model simulations—where wildfire and catchment characteristics were manipulated—indicated that increases in DOC were not linearly related to fire severity. Rather, the highest DOC loads occurred when the catchment was burnt at moderate severity, while the highest peak concentrations occurred at low severity. This work suggests that hydrological connectivity between the terrestrial and aquatic environment may be an important driver of post-fire responses in semi-arid watersheds, a new hypothesis that will be tested by further modeling and observations.

Integrated Modeling of Carbon and Nitrogen Cycling at the Yakima River Basin

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River corridors play important roles in watershed carbon and nitrogen cycling. This study seeks to quantify the cumulative impacts of river corridor hydrologic exchange flows, dissolved organic matter chemistry, and microbial activity on biogeochemical cycling. Leveraging the Advanced Terrestrial Simulator (ATS) and PFLOTRAN software coupled through the Alquimia interface from the IDEAS–Watersheds software ecosystem, the research team developed an integrated modeling framework that represents the river corridor as an integral part of a watershed using unstructured meshing in ATS. By seamlessly linking dynamic river flow processes and heterogeneous terrestrial inputs, such integrated modeling allowed for investigations into how variations in land use, hydrogeology, climate, and disturbances interact to control the spatial and temporal variability of aerobic respiration and denitrification processes across the Upper Yakima River Basin.

The research team further quantified the variability of organic carbon speciation and their impacts on carbon and nitrogen processing using Fourier-transform ion cyclotron resonance mass spectrometry measurements distributed across the Yakima River Basin. PFLOTRAN reaction sandbox was used to implement reaction networks and kinetics informed by carbon speciation and to scale up to watersheds. Model predicted discharge and aqueous concentrations of multiple species were confronted by observations collected at various locations to improve model parameters and process representations. Machine learning-based inverse

mapping was employed for model parameter estimation. This study not only highlights the feasibility of modeling watershed carbon and nitrogen cycling at a high mechanistic level, but it also demonstrates that intentional, two-way iteration between modeling and experiments accelerates knowledge advancement.

Harmonizing Multiple Information Sources to Predict River Corridor Respiration at the Watershed Scale

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Respiration in river corridors is an essential process by which organic matter is converted to CO₂ and released into the atmosphere. River corridors are also highly sensitive to changing climate conditions. Understanding the factors that control the location and timing of organic matter processing in river corridors is critical to predicting their role in climate feedback. Using a ModEx approach, the research team addressed this challenge in two ways: (1) evaluating a basin-scale model-generated hypothesis with field estimates of riverbed sediment respiration and (2) using model-generated sediment respiration hypotheses to quantify variations in spatial scaling.

Researchers conducted this work in the Yakima River Basin (YRB), which is representative of the environmental gradients in the larger Columbia River Basin. Process-based modeling predicted a consistent spatial pattern for respiration across the YRB: respiration rates increased with stream order, reaching an average maximum at fifth-order streams, then decreased toward the main Yakima River channel. Field measurements also revealed a similar spatial organization, although researchers observed the potential for maximum respiration in fourth-order streams. The team also found that sediment respiration makes up >98% of total respiration across all 48 field sites. Sediment respiration is, therefore, dominant in the river system. Still, spatial respiration patterns differ markedly between model predictions and other measurements of microbial processes (e.g., cotton strip experiments or lab incubations). These results indicate that existing models could be missing key processes and that prediction-observation mismatches can be used to guide further model development. From a spatial scaling perspective, the process-based model was used as a digital twin to

explore scaling relationships between sediment respiration and watershed area.

This study used variations in spatial scaling relationships as additional model-generated hypotheses that researchers could evaluate with their field respiration estimates. Specifically, predicted scaling relationships tend to be super-linear in more homogeneous landscapes with longer residence times when compared with more heterogeneous landscapes. On the other hand, predicted scaling behavior becomes more uncertain as human-influenced land cover increases. These hypotheses indicate a strong coupling between in-stream and hillslope processes, modulated by climate, vegetation, and land cover. Thus, scaling relationships represent simple quantitative hypotheses ripe for evaluation via ongoing ModEx, including independent testing through field measurements.

Alterations to Carbon, Nitrogen, and Phosphorous Biogeochemistry Across a Burn Severity Gradient: Implications for Varied Wildfire Impacts on River Corridor Hydro-Biogeochemistry

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In the Pacific Northwest, changes in wildfire regimes have highlighted the need to better understand how burned vegetation alters ecosystem nutrient dynamics. Char and ash runoff into waterways can change aquatic ecosystem function, and recent research has indicated these materials may be more bioavailable than previously considered. This study examined how wildfire influences carbon (C), nitrogen (N), and phosphorus (P) concentration and molecular composition in solid chars and their leachates to understand the amount and types of materials that could be transported to aquatic ecosystems post-fire. Using an open-air burn table, the research team generated vegetation-derived chars representing major ecotones in the Pacific Northwest (e.g., Douglas-fir forest, mixed conifer forest, mountain woodland, and sagebrush shrublands). Researchers manipulated the moisture and duration of heating when generating

the chars and evaluated the differences in burn severity that resulted, using field-derived metrics of burn severity (e.g., unburned, low, moderate, high).

Findings showed that total C and N concentrations generally decreased, while P increased with increasing burn severity in the solid chars. The percentage of C, N, and P mobilized to the aqueous phase showed contrasting patterns with burn severity. As burn severity increased, the percentage of soluble P systematically decreased regardless of vegetation type, while shifts in soluble C and N were related to vegetation type. Increasing burn severity also changed the molecular composition of both the solids and leachates. In the solid chars as burn severity increased, C chemistry became less diverse, aromatic six-member N structures were generated, and P was composed of proportionally more crystalline inorganic species as measured via X-ray absorption near edge structure and nuclear magnetic resonance. Leachate composition demonstrated a loss of protein-like compounds and an increase in aromaticity (measured via Fourier-transform ion cyclotron resonance mass spectrometry) with increasing burn severity. Overall, findings indicate that shifts in C, N, and P concentration and chemistry post-fire are related to burn severity. Thus, post-fire C, N, and P dynamics may uniquely impact downstream riverine ecosystem responses with shifts in landscape burn severities expected due to changing fire regimes.

Continental-Scale ModEx to Understand Sediment Respiration Using ICON Science

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In river corridors, sediments from the hyporheic zone can dominate channel metabolism, but it can also be a minor contributor, with literature estimates ranging from 4% to 96% of stream metabolism coming from the hyporheic zone. At present, no models can explain among-stream-reach variation in the hyporheic zone contribution to stream metabolism. This significant gap in river corridor science needs to be addressed to advance collective ability to understand and predict the future state of river corridor hydrobiogeochemical function (e.g., greenhouse gas emission rates). The research team approached this challenge with a continental-scale effort aimed at (1) producing knowledge

and models that are transferable and generalizable across diverse river corridor settings and (2) generating science outcomes, data products, and modeling infrastructure that is mutually beneficial across a broad range of stakeholders.

To achieve these goals, ICON science principles are being used to conduct an ongoing study that is integrated across disciplines, coordinated via use of consistent protocols, open throughout the research lifecycle, and networked with multiple stakeholders to understand and respond to diverse needs. Through globally open engagement prior to initiating the study, the research team received feedback and modified the study design so that project outcomes would be beneficial to as many stakeholders as possible. Initial engagement was followed by crowdsourcing samples across the contiguous United States, with sampling locations guided by machine-learning (ML) models. Resulting estimates of hyporheic zone respiration were used to test the ML models, update those models, and generate new ML-based guidance on where to sample next. This feedback between models and data generation is ongoing monthly, with significant changes to the spatial distribution of prioritized sampling locations. The engagement process is also approached as an iterative loop, with follow-on engagement in educational settings with direct student participation. Intentional use of ICON principles and iterative feedback between models and data are providing new opportunities for a broad range of researchers, offering unprecedented abilities to predict and understand hyporheic zone biogeochemistry, and generating FAIR products from which all can benefit.

Amplifying the Impact of the River Corridor Science Focus Area with ICON Principles

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Integrated, coordinated, open, and networked (ICON) science principles help projects design their work to intentionally meet goals that ultimately amplify impact. Integrating across disciplines and scales encourages diverse insights. Coordinating to use consistent protocols and methods enables transferability and synthesis. Being open and implementing findable, accessible, interoperable, and reproducible (FAIR) data principles throughout the research lifecycle promotes knowledge exchange. Being networked whereby research is designed and/or implemented with a broad range

of stakeholders facilitates mutual benefit with those beyond the immediate research team. ICON has been used in part of the River Corridor SFA (RCSFA) for several years, primarily as the foundation and guiding principles behind the Worldwide Hydro-biogeochemistry Observation Network for Dynamic River Systems research consortium, which has allowed the RCSFA to have a global reach through crowd-sourced, collaborative science.

More recently, ICON is being used across the whole RCSFA, with a goal of “ICONing” the entire project. Intentional integration in the RCSFA allows for effective use of the ModEx cycle, which amplifies the impacts of both the models and the measurements. For example, field locations for sediment respiration estimates were targeted across the Yakima River Basin (YRB) by using information from process-based model predictions. In another example, the SFA’s ICON-ModEx study intentionally integrates machine learning (ML), public data, and new biogeochemical, physical, and microbial sampling. Integrating across these disciplines enables application of the resulting ML models to the YRB.

To be coordinated and open, the RCSFA uses all applicable ESS-DIVE reporting formats to publish standardized, FAIR data. This project has seen data reuse from external groups for proposals and manuscripts attributed to following the rigorous reporting format requirements. The RCSFA also leads crowdsourced manuscript writing efforts, another example of being open, which drives new connections and external use of project data. One component of the RCSFA’s approach to being networked is engaging with scientists and educators from the Confederated Tribes and Bands of the Yakama Nation, a critical rightsholder in the YRB. These engagements build relationships and identify opportunities for mutual benefit. Together, the ICON principles are equipping the RCSFA to amplify its reach beyond the team, land, and science domains on which it has historically focused.

A Hypothesis-Driven ModEx Approach for Mechanistic Understanding of Hyporheic Zone Biogeochemistry

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The hyporheic zone plays a dominant role in channel metabolism and biogeochemistry for river corridor systems. Hyporheic sediment respiration often exhibits high spatial variability within and across river basins, imposing a substantial challenge for building transferable process representations in predictive models of river corridor biogeochemical

functions. This study used a hypothesis-driven approach that integrates theoretical knowledge generation, model development, and numerical experimentation to address this challenge. This approach allowed the research team to incorporate process information from new data and physical consistency with previously developed theories for more accurate and scalable biogeochemical predictions.

Building upon the team’s previous hypotheses regarding thermodynamic controls, returns on investment, and bioavailability that provide partial explanations for observed patterns in sediment respiration across continental scale, researchers further hypothesized that the biological and physical properties of hyporheic zone sediments modulate variations of sediment respiration rates. A numerical experiment showed low substrate accessibility significantly reduces the probability for a microbe to be surrounded by substrate, and thus decreases the effective organic matter concentration, leading to lower predictions of respiration rates. Similarly, increasing variations in microbial biomass among sites disproportionately generated wider distributions of predicted rates. Both numerical observations provided additional explanatory power for empirical distributions of rate measurements.

In addition, the modeling experiments provided new model-generated hypotheses that require specific data types to evaluate, such as microbial biomass and sediment grain size distribution that are readily available from the WHONDORS (Worldwide Hydro-biogeochemistry Observation Network for Dynamic River Systems) research consortium, thus furthering the hypotheses-driven ModEx cycle. This study illustrates the concept and application of hypothesis-driven ModEx in which each model-data hand off is based on and guided by specific hypotheses. This is distinct from traditional ModEx approaches that emphasize data assimilation.

Machine Learning Enables Computationally Efficient and Stable Integration of Genome-Scale Metabolic Networks with Reactive Transport Models to Predict Microbial Metabolic Switching

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Genome-scale metabolic networks (GEMs) provide a detailed view of microbial metabolism and its interactions

with the environment. In contrast with coarse-grained biogeochemical models, the high-resolution description of microbial processes in GEMs can help establish a molecular-level understanding of microbially driven biogeochemical cycles by incorporating high-throughput omics data. However, integrating GEMs with reactive transport models (RTMs) presents a challenge due to the significant computational burden caused by iterative implementation of linear programming (LP) to obtain flux balance analysis (FBA) solutions in each time and spatial grid during simulations.

To overcome this challenge, the research team developed a novel machine learning-based method that efficiently integrates FBA with RTM. The main breakthrough is to train artificial neural networks (ANNs) as a surrogate FBA model and use the resulting reduced-order FBA models as source and sink terms in RTM. The team's case study of the *Shewanella oneidensis* MR-1 strain demonstrates the effectiveness of the proposed method. The simulation of this organism's growth presents an additional challenge due to the intricate dynamics of metabolic switches among multiple substrates. During the aerobic growth on lactate, *S. oneidensis* produces metabolic byproducts (e.g., pyruvate and acetate), which are subsequently consumed as alternative carbon sources when the preferred ones are depleted.

No computational methods that allow for the simulation of such intricate dynamics by combining FBA (or its surrogate models) with RTM are currently available. The research team addressed this issue by adopting a cybernetic approach that predicts metabolic switches as the product of dynamic competition among multiple growth options. In both zero-dimensional batch and one-dimensional column configurations, ANN-based reduced-order models achieved a significant reduction in computational time, up to several orders of magnitude, compared to the original LP-based FBA models. Additionally, the ANN models generated robust solutions without the need for special measures to prevent numerical instability.

Due to such promising properties, the ANN-based FBA model developed in this work is currently integrated as a key component of CompLab, a recently developed Lattice Boltzmann-based modeling tool that simulates fluid flow and solute transport in porous media. This new capability will also be integrated into the MAGIEC (Metagenome Integration with Ecosystem Models) pipeline, which is being developed in collaboration with the KBase and IDEAS-Watersheds teams. Altogether, this work significantly improves ability to link molecular-level data and models with large-scale ecosystem modeling with enhanced computational efficiency.

Watershed Dynamics and Evolution Science Focus Area: Overview

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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). An integrated experimental, observational, and modeling program is proposed with the 9-year objective 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 program's 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. Also addressed are 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, the most intensively used freshwater resource region in the contiguous United States.

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

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Theme 1 in the Watershed Dynamics and Evolution SFA focuses on ecohydrology, biogeochemistry, and microbiology of nonperennial streams (dynamic headwaters) to evaluate the quantity and composition of water being transported from upland catchments into the stream network. The goal is to understand how variable saturation drives hydro-biogeochemical processes that influence downstream metabolism. Researchers will yield high spatially and temporally resolved data of surface flow in multiple headwater catchments that differ in land cover to inform numerical models describing flow in nonperennial streams, which will guide future field data collection. Researchers will also study surface and subsurface hydrology, plant water use, biogeochemical processes, and microbial community dynamics in a headwater catchment to capture how these processes respond to persistent or variable saturation. Field studies will be combined with laboratory investigations to understand how colloid and particle dynamics influence (micro)nutrient levels across saturation and redox gradients generated through intermittent flow. This project hypothesizes that highly dynamic redox-active zones in nonperennial stream channels contribute significantly to the export of carbon, nutrients, and trace metals to the downstream environment.

This research effort builds on expertise developed under the Critical Interfaces SFA that focused on biogeochemical transformations within streams. Microbial communities can rapidly respond to changing environmental conditions, as well as seasonal and episodic changes in flow, redox state, and nutrient availability. Such environmental changes control bioavailability of trace metals and may exert significant controls on the biosynthesis and function of metalloenzymes that are essential for many metabolic processes. Microbes have evolved various strategies to acquire essential trace

metals. Interactions between copper(II) and several other transition metals with the chalkophore methanobactin were characterized using spectroscopic methods. The complexation of metal ions by methanobactin occurs through several steps, including rapid coordination of metal ions to functional groups, conformational rearrangement, and formation of oligomers dependent on metal ion and stoichiometry.

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

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Within Oak Ridge National Laboratory's Watershed Dynamics and Evolution (WaDE) SFA, Theme 2 will characterize stream corridor processes at the reach scale using a combination of field experiments, laboratory mesocosm studies, and modeling. This work is motivated by the knowledge that mid-order streams are reactive conveyors that receive, process, and transport carbon, nutrients, and other solutes from upstream and the surrounding uplands. Furthermore, these mid-order streams are a vital link between low-order headwaters and larger rivers. Nevertheless, they are noticeably underrepresented in the research literature, so quantitative understanding of their roles in watershed function is lacking. These experiments and data analyses are designed to address specific questions and hypotheses related to (1) quantifying the contributions of water column gross primary production and ecosystem respiration to net ecosystem production 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 gross primary production and ecosystem respiration to disruption by transient high-flow events.

To address these research focuses, scientists will establish three long-term observation stations in the Theme 2 research watershed, the location of which will be selected to coincide with dominant land cover categories in the region. Each station will be equipped with multiparameter sondes, including dissolved O₂ and CO₂ sensors, as well as pressure transducers in stilling wells to measure and record high-temporal resolution water quality and discharge data. Observations and experiments will be tiered in spatial and temporal scale from individual bottle experiments (hours) to laboratory flume experiments (weeks to months) to long-term observation records in the field (months to years). Experimental design will be informed by data from WaDE SFA Theme 1 and

provide results used in Theme 3 (please see accompanying posters). The Theme 2 team will collaborate with microbiologists and microbial ecologists to inform data interpretation and analysis. Additionally, data will be used to inform development of a virtual watershed, which will be applied to data interpretation and the design of new experiments.

Watershed Dynamics and Evolution Science Focus Area Theme 3: Network Function—Understanding the Role of Heterogeneous Land Cover and Hydrologic Regimes on Stream Hydro-Biogeochemical Function Within and Across Mid-Order Watersheds

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Anthropogenic activities are altering watershed hydrology and land use and land cover with cascading effects on the storage, processing, and transport of water, nutrients, carbon, sediments, metals, and contaminants from watersheds. Theme 3 of Oak Ridge National Laboratory's Watershed Dynamics and Evolution (WaDE) SFA seeks to resolve the network-scale organizational controls on the emergent patterns and regimes in stream function along and across mid-order stream networks with heterogeneous land cover. Stream metabolism will serve as a key indicator of ecosystem function given its fundamental role in carbon and nutrient cycling and dependency on multiple parameters that are controlled by watershed structure, land cover, and hydrologic state. Specifically, Theme 3 will evaluate how stream metabolism and associated measures of stream function vary along the network and reflect connectivity between the stream and a mosaic of different land covers. This objective requires an understanding of (1) how complex interactions between watershed structure, land cover, and hydrologic state control emergent patterns in stream metabolism; (2) how these network-scale patterns align with fine-scale understanding of process dynamics; and (3) what resolution of system characterization is needed to accurately predict stream metabolism at any given scale.

This presentation will provide an overview of (1) the project-wide approach for determining representative

clusters of mid-order watersheds within the Tennessee River Basin and selecting three increasingly divergent watersheds across which to systematically translate, apply, and refine the process understanding and modeling capabilities gained over the next 10 years; (2) the Theme 3 network-scale investigations planned over the next 3 years; and (3) how these investigations integrate with parallel activities focused on:

- Water and solute mobilization and export from uplands with heterogeneous land cover (WaDE SFA Theme 1).
- Resultant feedbacks between flow, solute concentrations, and the resistance and resilience of stream function in stream corridors (WaDE SFA Theme 2).
- Development of a virtual watershed capability (WaDE SFA Modeling Crosscut).

Watershed Dynamics and Evolution Science Focus Area Modeling Crosscut: Model-Data Integration Strategies for Stream Metabolism Studies

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Conservative and reactive tracer tests, laboratory experiments, and continuous stream chemistry measurements are among the techniques available to characterize stream hydro-biogeochemical function. The Watershed Dynamics and Evolution SFA is developing and testing approaches and software to aid in the interpretation of those measurements, with a focus on stream metabolism. In particular, a novel multiscale model (Painter 2018) for transport in stream corridors is being combined with uncertainty-aware estimation of model parameters through Bayesian inference and the Markov chain Monte Carlo algorithm. Previous research showed that jointly interpreting tracer data from multiple observation points or different biogeochemical experiments increases the reliability of parameter estimates (Rathore et al. 2021; Rathore et al. 2022; Le et al. in review). Models can also be essential in evaluating experimental designs and assessing potential for system mischaracterization, as demonstrated by Rathore et al. (in review), for photosensitive tracers as a strategy to separate hyporheic and surface storage zone effects. This research extends those parameter identifiability studies to include stream metabolism models. A stream metabolism model was implemented into the PFLOTRAN software and combined with the project's multiscale stream corridor model in the Advanced Terrestrial

Simulator to construct a reach- to watershed-scale reactive transport model for dissolved oxygen dynamics. Using the Modeling Crosscut team's reactive transport model, scientists performed numerical experiments to interpret synthetic dissolved oxygen time series through Bayesian inverse modeling under different relative contributions of gross primary productivity, ecosystem respiration, reaeration, and groundwater exchange to study parameter uncertainty and identifiability. These insights are helpful for designing data collection campaigns aiming to characterize stream metabolic function. Furthermore, the workflow tools developed will be used to analyze new measurements as they become available.

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Rathore, S. S., et al. 2021. "On the Reliability of Parameter Inferences in a Multiscale Model for Transport in Stream Corridors," *Water Resources Research* **57**(5), e2020WR028908. DOI:10.1029/2020WR028908.

Rathore, S. S., et al. 2022. "Joint Estimation of Biogeochemical Model Parameters from Multiple Experiments: A Bayesian Approach Applied to Mercury Methylation," *Environmental Modelling & Software* **155**, 105453. DOI:10.1016/j.envsoft.2022.105453.

Rathore, S. S., et al. "Numerical Evaluation of Photosensitive Tracers as a Strategy for Separating Surface and Subsurface Transient Storage in Streams." In review.

Watershed Functional Traits from Bedrock-to-Canopy Regulate the Retention and Release of Nitrogen Within Mountainous Watersheds

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Mountainous watersheds are characterized by extreme variance in functional traits such as vegetation, topography, lithology, and geomorphology, which together play critical roles in determining nitrogen (N) retention and release. This research parses out the role different watershed traits play in cycling N at the hillslope and the catchment scale.

At the hillslope scale, researchers worked along a montane hillslope underlain by N-rich marine shale and quantified organic and inorganic nitrogen pools in soils, porewater, vegetation, microbial biomass, and derived from shale weathering products. The major sinks for N along the hillslope include vegetation (~13 kg m⁻², roots + shoots) and soils (~3.5 kg m⁻²: 0.68–6.8 kg m⁻²). While a portion of the mobile nitrogen, such as nitrate (NO₃⁻), translocates from the hillslope to floodplain soils and the groundwater, a significant fraction is lost *in situ* through gaseous pathways as the water table ascends and recedes through hillslope soils. Nitrate stable isotope systematics show the concomitant enrichment of both δ¹⁵N_{NO₃} and δ¹⁸O_{NO₃} within the weathering zone of the hillslope, accompanying a drop in NO₃⁻ concentrations. Moreover, the accumulation of nitrous oxide (N₂O), simultaneous with isotopic enrichment, suggest denitrification is likely responsible for gaseous NO₃⁻ loss. Interestingly, N₂O fluxes at the soil surface are negligible (-3.7±2.4 g m⁻² yr⁻¹), indicating a strong sink for N₂O (to N₂) between the weathering zone and atmosphere.

At the catchment scale, researchers compared two representative but contrasting catchments that differ markedly in total NO₃⁻ export. Coal Creek is underlain by granitic rock and sandstone, with a conifer-dominated land cover, while seven kilometers away, the East River has a diverse vegetation cover, sinuous floodplains, and is underlain by N-rich marine shale. However, the N-cycles of these catchments differ starkly. The stable isotope ratios of NO₃⁻ (δ¹⁵N_{NO₃} and δ¹⁸O_{NO₃}) demonstrated that conifer-dominated Coal Creek retained nearly all (~97 %) atmospherically deposited NO₃⁻. By contrast, the East River showed stronger biogeochemical processing of NO₃⁻ prior to export. The conservative N-cycle within Coal Creek is likely due to the abundance of conifer trees and a smaller riparian region, retaining more NO₃⁻ overall and reduced processing prior to export. The East River catchment is a strong hotspot for nitrogen cycling, with NO₃⁻ reduction at the soil-saprolite interface and within the floodplain, buffering the export of NO₃⁻.

These studies aim to highlight the value of integrating isotope systematics to link watershed functional traits to mechanisms of watershed element retention and release—an endeavor that becomes more important in the face of changing climate.

Emergent Controls on Microbial Functional Distributions Across a Mountainous Watershed

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Watershed traits including topography, vegetation, and soil characteristics are shaped by interacting climate and geologic variability in mountainous watersheds. Energy resources are constrained by these interacting watershed traits, and water availability is central in selecting microbial biogeochemical function. By understanding how watershed traits influence the spatial distribution of microbial functional traits, this research aims to predict how changes in watershed traits influence hydro-biogeochemical process response to disturbance. Researchers have quantified the spatial distribution of genome-inferred microbial functional traits for over nine field campaigns (20 watershed locations). From 724 metagenomes, 91K species were identified, as well as exceptional virus diversity. A database of inferred microbial functional traits has been established using new computational workflows. Machine learning is being used to scale and predict microbial trait distributions to uncover relationships with watershed traits quantified by remote sensing. For example, plant canopy height, leaf mass per area, and elevation are the best predictors of the genomic capacity for nitrogen-mobilizing ammonia oxidation, a process carried out primarily by ureolytic Thaumarchaeota. By contrast, the genomic capacity for nitrate retention (i.e., dissimilatory nitrate reduction to ammonia versus denitrification) is higher in topographic depressions that are occupied by willow shrubs across the watershed. This extends upon observations of floodplains as key nitrogen retention control points. Intensive studies are being completed at finer scale across space (e.g., soil-to-bedrock profiles) and time (e.g., floodplain inundation). For example, shale weathering contributes to both carbon and nitrogen exports, and mycorrhizal fungi have also been observed colonizing tap roots of sagebrush in bedrock fractures 2 m below the surface and may contribute to weathering. Methane off-gassing from Mancos shale bedrock may be an important carbon source in the subsurface of upland soils, evidenced by high gene expression of methane oxidizing Actinobacteria in

deep soils and negligible methane fluxes from the soil surface. In surface soils, topography and plant roots interact to create anoxic soil microsites that contribute to soil carbon stabilization and greenhouse gas emissions. In floodplains, methane production is driven by highly fluctuating river discharge; however anaerobic methane oxidation coupled with nitrate reduction may be an important control on overall methane fluxes. These finer scale studies form the basis of mechanistic understanding of microbial influence on biogeochemical cycling from bedrock-to-canopy, and combined with this project's watershed scale surveys, are informing targeted field sampling campaigns, coupled laboratory experiments, and model development to predict watershed responses to future disturbance.

Identifying Sources of Stream Water Based on Stable Water Isotopes and Hydrologic Models

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Identifying dynamic stream water contributions from the snowpack versus monsoonal rainfall is crucial to understanding potential changes in water resources in a changing climate with reduced snowpack. Using data from 81 snow pits collected over 5 years across the East River watershed, scientists investigated the temporal and spatial variation of the snowpack stable isotope ratios. These data showed that snow sublimation and melt-freeze redistribution led to isotopic enrichment with more intense fractionation at lower elevation. The snowpack isotopes were used together with LiDAR snowpack observations to couple a hydrologic and a snowpack isotope model to assess controls on isotopic inputs across the East River catchment.

Results showed that the most depleted isotope conditions occurred in the upper subalpine where snow accumulation was high, and rainfall was low. Energy and snow-availability determined the snowpack's isotopic fractionation, which was highest where vegetation shading was low (i.e., above treeline and grass and Aspen-dominated portions of upper montane). Scientists used the precipitation isotope inputs to the East River catchment to investigate the partitioning of snow and rainfall into evapotranspiration (ET) and summer and nonsummer discharge via isotope mixing analyses. Results showed that one third of the snow partitioned to ET and 13% of the snowmelt sustained summer streamflow. Only 8% of the rainfall contributed to the summer streamflow, because most of the rain (67%) partitioned to ET.

Catchments with higher tree cover demonstrated a higher share of snow becoming ET and less summer streamflow. Finally, physically based integrated hydrologic model simulations with dynamic-flux particle tracking showed a strong linear trend with the isotope mixing analysis for the fraction of ET coming from rain versus snow ($R^2=0.88$), suggesting the simulation captures key functional dynamics of water partitioning to ET. However, simulated discharge from snow exceeds that of the amount estimated from the isotope observations, suggesting either an underestimation of simulated ET and/or a limitation of the endmember analysis to account for groundwater storage changes.

The isotope data further enabled scientists to relate isotopically distinct high elevation snowmelt to stream water isotope dynamics. Results showed that stream water isotopes can serve as a catchment integrated signal of high elevation snowmelt contributions to stream discharge. Interannual variation of the stream water isotopes could serve as an early warning signal for a shift towards reduced high elevation snowmelt contribution to the catchment runoff.

Is Groundwater Effective at Buffering Mountainous Watersheds in a Changing Climate?

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A synthesis of western U.S. snowpack projections reveals that ongoing declines of snow are expected to continue in the coming decades, yet little is known about how groundwater buffers watershed function, including water yields, as the climate transitions to a “low-to-no snow future.” Highlighted are the results of that synthesis, as well as numerical and *in situ* studies examining the sensitivity of interannual variability of snowpack changes in the East River of the Upper Colorado River Basin with the aim to better understand groundwater dynamics given the feedbacks between snow, soil moisture, and groundwater. Observations of environmental tracers (e.g., dichlorodifluoromethane, sulfur hexafluoride, tritium, and helium-4) are used to estimate groundwater residence times, suggesting a mixture of modern and premodern water ages (decades to millennia), necessitating a binary mixing residence time model to represent the bedrock dynamics.

Dissolved noble gas analysis shows that groundwater recharge is preferentially generated at high watershed elevations. Additionally, results of tritium from a new hillslope weir network co-located with a soil moisture campaign suggest headwater runoff consists of water ages ranging from 10 to 70 years, highlighting the importance of groundwater flow feeding near-source surface flow. Numerical hillslope modeling suggests that long residence time bedrock groundwater can represent a considerable flux into the shallow soil and floodplain systems, and that the partitioning of young residence time water from snowmelt versus old groundwater is sensitive to the bedrock hydrogeologic parameters. These results highlight the need to better characterize bedrock systems to improve understanding of the connectivity between groundwater flow paths and shallow soil and surface waters.

Finally, watershed-scale simulations indicate that lateral subsurface flow is a critical mechanism moving snowmelt downgradient to generate streamflow, subsidize evapotranspiration, and maintain groundwater levels in water-limited portions of the basin. Simulations indicate exceptionally warm and dry water years in the last decade have initiated significant groundwater declines. Additional warming will exacerbate storage loss through increased forested water use, with streamflow reductions 20% to 60% larger when accounting for depleted groundwater reserves. Researchers estimate groundwater destabilization in a warming climate that is unable to rebound to historical levels with a significant impact on streamflow. Ongoing hydrologic observations (e.g., snowpack, soil moisture, groundwater levels, streamflow) coupled with a comprehensive campaign evaluating groundwater ages at the East River will help to inform model experiments to determine the role of groundwater buffering in mountainous systems.

Synthesis of Hydrological Science in the East River from Evapotranspiration Estimates to Long-Term Climate Dynamics

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Watershed hydrological behaviors are fundamental to its functions. Quantifying the water fluxes moving across interfaces of compartments of the hydrological cycle is key to understanding and predicting its functions. Evapotranspiration (ET) moves a large quantity of water across the land–atmosphere interface and often contributes most to uncertainties of hydrological behavior. Accurate quantification of ET is a fundamental challenge in predicting watershed hydrological function. Two aspects of this ET research are highlighted: ET uncertainty quantification across different methods and a historic trend of ET behaviors.

Two major factors contribute to ET uncertainties and difficulties among different methods: unknown true ET values for benchmarking and differences in meteorological inputs, ET formulations, and parameterization. Understanding sources of uncertainty and developing gold standard benchmarking platforms and datasets are key to accurately predicting ET at watershed scales and beyond. For ET synthesis, a concerted effort was conducted to synthesize ET-related research across the Watershed Function SFA. Some key progresses from this effort are highlighted, including the development of ET benchmarking platforms and datasets using a controlled lysimeter setup and its use to improve ET model parameterization, as well as the comparison of various ET methods at selected benchmark locations and time periods to identify sources of uncertainties. Results from this effort suggest (1) up to >50% variations of ET quantity across the different methods, particularly in the summer growth season; (2) non-linear and scattered correlations of time-stamped ET across different approaches suggesting fundamental deviations among these approaches, and (3) meteorological forcing (e.g., radiation and wind) is a significant contributor to variations across the approaches. A few key improvements are also identified to improve ET quantification at the East River watershed.

For historic ET analysis, a statistical time series analysis (1966 to 2021) was applied to 17 locations at the East River watershed. ET was calculated using the Budyko model, Thornthwaite and Hargreaves equations, and the Penman-Monteith equation. The results were used to calculate standard precipitation index and standard precipitation–evapotranspiration index. Analysis suggests shifting of more locations toward water-limited scenarios, with these water-energy limitation zonation patterns driven by dynamic climatic processes. This provides a historic context for these observations of changes to ecosystem properties and function.

Community Research Activities to Support Mountainous Hydrology at the East River Watershed

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The research supported by DOE's ESS program through the Watershed Function SFA at the East River watershed has served as a hub and catalyst for a myriad of complementary research projects to advance the science of mountainous hydrology. Major investments from other BER programs—including ARM program's deployment of an atmospheric observatory as part of the Surface Atmosphere Integrated Field Laboratory (SAIL) campaign and the Atmospheric System Research program's support for science using SAIL—have enabled North America's most comprehensive atmosphere-through-bedrock mountainous field data collection location.

Recently, the Watershed Function SFA has catalyzed field research activities to fund advanced connectivity development and novel precipitation sensing methods funded by the Advanced Scientific Computing Research program in the area, which build upon a decade-plus of ESS investments to its cohort of university investigators. Other federal investments leveraged from DOE's investments include NOAA's efforts to advance weather and forecasting with the deployment of additional atmospheric instrumentation with the Study of Precipitation, the Lower Atmosphere and Surface for Hydrometeorology (SPLASH) and NSF's Sublimation of Snow (SOS) campaign and Critical Zone Collaborative Network (CZCN). Together, these far-ranging observational datasets are sensitive to dominant atmospheric, terrestrial, and subsurface processes, and their interactions that determine how mountainous watersheds retain and release

water and solutes. They also provide insights into how a changing hydroclimate might impact those processes.

This poster highlights ongoing research and connections between the Watershed Function SFA, SAIL, SPLASH, SOS, CZCN, and the recent DOE workshop on “Understanding and Predictability of Integrated Mountain Hydroclimate.” Connections also span across other community activities including snowflakes measured by SAIL and snowpack measured by the Airborne Snow Observatory (ASO). Aerosols measured by SAIL impact both snow albedo and nutrients as measured by ASO and Watershed Function SFA field observations focused on connecting said processes to surface and subsurface processes and eventual riverine export. The diversity of datasets collected in the East River watershed presents opportunities for researchers and points to the need for approaches, as highlighted in the workshop report on integrated mountain hydroclimate, that close spatiotemporal observational gaps and provide critical benchmark data for up- and down-scaling approaches and ModEx workflows. With such capability, the benchmark data collected at the East River watershed can interrogate and ultimately improve atmosphere-through-bedrock process model simulations, such that those models enable the transfer of knowledge derived in the East River watershed to other mountainous watersheds in the Upper Colorado River Basin.

Investigation of Environmental Factors Driving Shifts in Vegetation Health and Functional Traits Across the East River and Taylor Watersheds

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Forest decline due to pulse and press disturbances—including bark beetles, temperature increase, earlier snowmelt, exceptional droughts, and wildfire—have been observed in mountainous ecosystems, affecting species diversity and composition, associated functional traits, productivity, and mortality. To better understand how forested regions of watersheds will respond to future perturbations, it is critical to quantify and characterize such ecosystem

changes. This work performed a multidecadal analysis of satellite data spanning 35 years to capture changes in vegetation health and plant traits that occurred over the East River and Taylor watersheds in the Upper Colorado River Basin. Landsat images were used to compute a multiyear trend of vegetation health based on normalized difference vegetation index (NDVI). Also used was a new remote sensing index for leaf mass per area (iLMA) recently developed to map the spatiotemporal variation in LMA.

Covariability analysis with geomorphological and climatic properties shows that the response to disturbance in trees, shrubs, and meadow plants is heterogeneous across the elevation and geological gradients. Specifically, decline in productivity was observed in lower subalpine regions (2800–3200 m)—areas of transition between water and energy limitation—where increasing drought stress may be more evident. Areas of decreasing productivity are also associated with south-facing slopes. Among tree species of Aspen, Engelmann spruce, Subalpine fir, and Lodgepole pine, about 45–65% of forest area in the East River was associated with decrease in canopy health, with Aspen forest being affected to a greater extent. Increased productivity was observed at higher elevations spanning subalpine and alpine regions (3400–3600m). LMA shows an average loss of about $5\text{g}^*\text{m}^{-2}\text{yr}^{-1}$, mostly driven by changes in evergreen forests, and declining LMA with elevation. Bedrock properties also show heterogeneous relationships to plant productivity. For example, forests have shown an increased productivity at higher elevation over shale and granodiorite bedrock, unlike those on alluvium that followed an average negative NDVI trend.

Further, time-series clustering and correlation analysis of meteorological forcing across the domain shows the importance of climatic variables, such as air temperature, measured and computed across 17 meteorological stations. This supports the hypothesis of changing water and energy balance being linked to increased productivity at higher elevations. Climate-driven changes in vegetation performance directly impacts ecosystem biogeochemical processes and microbial catalysts that alter, for example, the retention of soil nutrients, and may underlie multidecadal changes in nitrogen export observed in the East River.

Predicting the Aggregate Hydro-Biogeochemical Response of Mountainous Watersheds Across Scales and Subsystems

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Reactive Transport Models (RTMs) are crucial to improve scientists' ability to predict the hydro-biogeochemical response of watersheds. However, these models must be able to accurately represent the complex multiscale, multiphysics processes that occur in watersheds. A scale-adaptive reactive transport modeling approach that involves using distinct codes was implemented to capture processes at the appropriate scale across watershed subsystems. In the subalpine and upper montane regions, the Copper Creek subcatchment was studied as a test case to understand how seasonal and interannual climate variability affects the observed relationship between the volume of water flow and solute concentrations (Xu et al. 2022). A Pumphouse lower montane (PLM) hillslope transect, established across a representative lower montane system, in turn, was used to disentangle the complex interplay between physical, geochemical, and biological processes controlling long-term chemical weathering of shale, with a focus on microbial aerobic respiration and changes in nitrogen stocks and fluxes resulting from snowpack variability (Stolze et al. 2022; Arora et al. in preparation). Hydro-biogeochemical exchange functions in the floodplain were also used to understand subsurface biogeochemical exports and their effects on river chemistry (Dwivedi et al. in preparation). The Lower Triangle region (LTR) of the East River is unique, as its hydrology is dominated by discharge from upstream subcatchments such as the Copper Creek and comprises interacting hillslope and floodplain subsystems (Özgen-Xian et al., 2020, 2023). As such, this system was used to integrate understanding developed across subsystems. The complex reaction network from the PLM hillslope transect and floodplain subsystems was used to capture nitrogen dynamics in LTR. The resulting model is being used to quantify the uncertainties associated with meteorological forcings, evapotranspiration, and subsurface flow and how they affect the aggregate hydro-biogeochemical response of the East River watershed.

Arora, B., et al. "Changes in Plant Productivity and Nitrogen Fluxes in a Mountainous Watershed as Affected by Snowpack Decline in Recent Decades." In preparation.

Dwivedi, D., et al. "Developing Insights into River Corridor and Watershed Hydro-Biogeochemistry Across Scales." In preparation.

Özgen-Xian, I., et al. 2020. "Wavelet-Based Local Mesh Refinement for Rainfall–Runoff Simulations," *Journal of Hydroinformatics* **22**(S), 1059–1077. DOI:10.2166/hydro.2020.198.

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Importance of Meander to Reach-Scale Heterogeneity in Stream Chemistry Changes

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Understanding river corridor biogeochemical function and scaling up that understanding to watershed scale requires an understanding of the functional traits within the river corridor and how they interact to control river chemical outputs. Hypothesized important traits that have been investigated in the East River system are relief, bedrock composition, meander morphology, and the composition of intrameander sediments. The impact of these traits has been evaluated at the single meander (10s of m), short-reach (~1 km), and long-reach (10s of km) scale. At the long reach scale, Arora et al. (2020) identified bedrock composition as a key trait with higher solute concentrations in the shale-dominated upper reach as compared to a granodiorite-dominated reach. River water constituents derived primarily from shale included calcium, dissolved inorganic carbon, dissolved organic carbon, magnesium, molybdenum, nitrate, and sulfate ions. However, the ultimate exports to the river were controlled by coupling with other traits in a chemical species-specific way. For example, Fox et al. (2022) showed that intrameander floodplain sediments mediated export of hillslope shale-derived sulfate to the river through sulfate redox cycling coupled with river hydrologic stage. The importance of river stage coupling with intrameander

sediments was also shown in the case of nitrate. Dwivedi et al. (in preparation) showed that the rising limb has the highest denitrification potential, followed by the base flow and recession limb. Additionally, meanders with larger amplitude exhibited higher denitrification potential due to longer lateral flow paths through intrameander sediments. However, highlighting the challenge of scaling, Fox et al. (in preparation) showed that river chemistry changes due to lateral hyporheic exchange were concentrated at key locations along apparently geomorphologically similar river reaches. The locations of these disproportionate solute inputs stayed the same year over year, were independent of discharge magnitude, and were likely due to the largely stable texture structure of the meander sediments. However, discharge magnitude did impact the magnitude of solute inputs, with extreme discharge years, high or low, showing greater solute inputs than average years. Taken together, these studies highlight how the coupling of traits leads to emergent behavior observable at the river corridor scale and provide insights into how increased hydrologic variability will impact river water chemistry. They also demonstrate that detailed trait characterization (e.g., textural structure) is important for accurate scaling.

Science Focus Area Data and Wireless Communications Infrastructure Enabling Data-Field and Data-Model Integration

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The Watershed Function SFA project generates large, heterogeneous datasets at its East River field site that include hydrological, geochemical, geophysical, vegetation, microbiological, and remote sensing datasets. Field data is collected by the project team and collaborators, wireless sensors, and external sources (e.g., the U. S. Geological Service and the USDA’s Natural Resources Conservation Service). Researchers will present the SFA’s data and wireless communications infrastructure that addresses the challenges associated with environmental data acquisition, curation, quality analysis (QA), quality control (QC), integration, visualization, and download.

The SFA data management framework provides infrastructure and services to support various aspects of the project’s

data lifecycle. It establishes wireless connectivity for sensors in the field, performs automated quality checks of sensor datasets, and enables integration of diverse time-series data for use in analysis and models. The framework also includes tools for data management, preservation, discovery, and visualization. Sensor and geochemical data from the SFA project have been curated in a queryable database since the start of field observation efforts at the East River. A statistical QA/QC workflow is applied to priority meteorological, hydrological, and geochemical data streams. Machine learning (ML) and statistical algorithms are being explored to conduct basic screening of incoming data in near real-time for early detection of sensor malfunctions. An open source brokering service tool BASIN-3D (Broker for Assimilation, Synthesis and Integration of eNvironmental Diverse, Distributed Datasets) enables on-demand integration of diverse time-series datasets into a common format based on the Open Geospatial Consortium’s observations and measurements standards. The software has also been used to integrate data for ML applications and can be used to support other data streams in the future.

In order to facilitate real-time data streams from the field, researchers deployed an advanced wireless communication system at the East River field site in partnership with the DOE’s Energy Sciences Network user facility. The system leverages Starlink and 5G Citizens Broadband Radio Service technology to create a standalone, private cellular network. Low power 5G hubs in the field connect to this network and provide local sensor connectivity over Wi-Fi, long range radio, and Ethernet. For this pilot, researchers demonstrated real-time imagery, as well as live data transfers from a wireless network of distributed snow and soil temperature sensors. The combined systems, workflows, and tools are used for building crosscutting data products needed for hypothesis testing and numerical modeling of hydrological and biogeochemical processes in the East River watershed. It adopts a holistic view for data collection, assessment, and integration, which dramatically improves the products generated and enables a codesign approach wherein data collection is informed by model results and vice versa.

The Argonne National Laboratory Subsurface Biogeochemical Research Program Science Focus Area: Wetland Hydro-Biogeochemistry

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<https://ess.science.energy.gov/anl-wetland-sfa/>

<https://www.anl.gov/bio/project/subsurface-biogeochemical-research>

Within wetlands, water movement and biogeochemically catalyzed transformations of its constituents determine the mobility of nutrients and contaminants, emission of greenhouse gasses into the atmosphere, carbon (C) cycling, and water quality itself. The long-term objective of the Argonne Wetland Hydro-Biogeochemistry science focus area (SFA) is the development of a mechanistic understanding and ability to model the coupled hydrological, geochemical, and biological processes controlling water quality in wetlands and the implications of these processes for watersheds commonly found in humid regions of the United States. To accomplish this, the Argonne Wetland Hydro-Biogeochemistry SFA focuses research on a riparian wetland within Tims Branch at the Savannah River Site. Tims Branch contains riparian wetlands representative of those commonly found in humid regions of the Southeast that have C-rich soils and high iron (Fe) content. However, it is unique in that parts of the watershed received large amounts of contaminant metals and uranium from previous industrial-scale manufacturing of nuclear fuel and target assemblies. Groundwater and surface water level monitoring wells have been installed to provide hydrological context (e.g., gaining versus losing stream conditions) to the study sites within the watershed. Understanding the function of wetlands in relation to hydrologic

exchange, including the concentration of nutrients and contaminants within the soluble and particulate components of groundwater and surface waters, addresses the goal of the ESS Program to advance a robust, predictive understanding of watershed function.

The overarching research hypothesis is that hydrologically driven biogeochemical processes that create redox dynamic conditions from the nanometer to meter scales are major drivers of groundwater and surface water quality within riparian wetland environments. Researchers identified three major components, or focus areas, of the Tims Branch riparian wetland that represent critical zones containing hydrologically driven biogeochemical drivers that control water quality: sediment, rhizosphere, and stream. Within these three focus areas, researchers identified two common thematic knowledge gaps that inhibit the ability to predict controls on water quality: (1) in-depth understanding of the molecular-scale biogeochemical processes that affect Fe, C, and contaminant speciation within the wetland sediment, rhizosphere, and stream environments and (2) in-depth understanding of hydrologically driven biogeochemical controls on the mass transfer of Fe, C, and contaminants within wetland sediment, rhizosphere, and stream environments. Holistically addressing hypotheses related to these two knowledge gaps organizes the SFA in its development of a hydro-biogeochemical conceptual model of the Tims Branch riparian wetland.

Speciation of Iron and Uranium in Sediments Collected at Savannah River National Laboratory

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<https://www.anl.gov/bio/project/subsurface-biogeochemical-research>

The M Area Fuel Fabrication Facility at the Savannah River Site manufactured nuclear fuel and target assemblies between 1954 to 1989, resulting in significant discharge of uranium and co-contaminants (e.g., nickel, chromium, zinc, and lead) into Tims Branch (a small second-order stream) and associated riparian wetlands. The natural processes occurring in these environments are complex and control elemental dynamics through various reactions, such as adsorption, precipitation, and particle transport.

The Argonne (ANL) Wetland Hydro-biogeochemistry SFA focuses on providing the molecular-level information for relevant biogeochemical reactions to enable their inclusion in predictive models of the system. To better understand the redox dynamics in wetland sediments researchers collected ~30 cores from saturated and unsaturated locations along Tims Branch and characterized them at the Advanced Photon Source. Iron (Fe) and uranium (U) were primarily in their oxidized forms in near-surface sediments that remained dry. In below-surface, organic-rich areas of saturated sediments, researchers found reduced Fe species that are present in clays, oxides, and associated with organic matter. Uranium found in the same areas was reduced to U(IV) in the form of adsorbed complexes (i.e., not mineralized). Molecular U(IV) species are not yet described in thermodynamic databases and therefore not considered in transport models. This disconnect between modeled and actual species is likely to cause significant uncertainties in the predicted behavior of U in such environments. The dynamic redox nature of wetlands further complicates predictive understanding of the system—in gaining stretches of the stream, the Fe(II) in emerging groundwater oxidizes to form visible orange flocs, which Fe extended X-ray absorption fine structure spectroscopy determined to be composed of ferrihydrite and lepidocrocite. The oxides and contaminants found in these Fe flocs can experience redox transformations, which will affect their stability and transport as particles and as dissolved species. In addition to characterizing the flocs collected at the field site, researchers are also carrying out incubation experiments in the laboratory to determine the molecular speciation of Fe and the contaminants under alternating redox conditions (see ANL SFA poster by O’Loughlin et al.).

Transport and Accumulation of Uranium in a Fluvial Wetland: Importance of Hydrology and Colloids

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<https://www.anl.gov/bio/project/subsurface-biogeochemical-research>

A nuclear fuel fabrication facility released 43,500 kg of uranium (U) into a riparian wetland located on the Savannah River Site, South Carolina, between 1955 and 1988. Studies were undertaken to evaluate hydrology, geochemical processes, and suspended colloids on U accumulation in the wetland. Gamma radiation mapping surveys were conducted by systematically walking over the contaminated wetland with backpacks equipped with global positioning systems and sodium iodide gamma detectors. Based on maps compiled from >700,000 gamma spectra and eight sediment U depth profiles, it was determined that 94% of the released U remained in the wetland. The U in the wetland is concentrated in five multihectare areas along the stream, accounting for ~11% of the land area adjacent to the stream.

While land type (upland or wetland) and topography provided a reasonable first approximation of where much of the U was deposited, hydrological watershed modeling revealed that the stream velocity was especially slow through the accumulation areas. Using autoradiography combined with scanning electron microscopy–energy dispersive X-ray measurements of contaminated sediments, surprisingly few hot particles were detected. Instead, U was evenly distributed throughout the sampled sediment, suggesting that soon after release into the wetland dissolved U had bound to sediment particles that became suspended and later deposited in low energy (low flow velocity) portions of the stream and floodplain.

Iron (Fe) extended X-ray-absorption fine-structure (EXAFS) measurements of the colloidal particles (three size fractions between 3 kDa and 0.1 μm) indicated that they

consist predominantly of ferrihydrite and a smaller fraction of organic matter-bound Fe(III), without significant differences between groundwater and surface water colloids. Uranium L_{III}-edge EXAFS indicated that the U atoms in the larger colloids were predominantly associated with the mineral fraction as inner-sphere complexes (U-Fe distance of 3.44 Å). These studies show that wetlands can be extraordinarily effective at binding and retaining U, thereby providing a natural barrier to the transport of U out of a watershed. However, significant anthropogenic or climatic changes to wetlands, such as those associated with flooding, forest fires, or land use, may disrupt the complex hydrological and biogeochemical balance necessary to maintain long-term immobilization of U.

Modeling Hyporheic Zone Fe-S-C Cycling with “Cryptic” Sulfur Reactions at the Tims Branch Riparian Wetland (Argonne Wetland Hydro-biogeochemistry Science Focus Area)

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Tims Branch is a riparian wetland in the Savannah River Site, SC with uranium (U) contamination. U mobility is affected by iron (Fe) redox chemistry, which depends on interactions with carbon (C) and sulfur (S) in the hyporheic zone. Predicting Fe-S-C cycling is difficult not only because of variable redox gradients that develop in response to dynamic fluxes, but researchers hypothesize that it is further complicated by “cryptic” S cycle reactions not usually represented in reactive transport models. Researchers have found that model simulations at Tims Branch with standard redox reactions (no “cryptic” S reactions) struggle to capture the observed persistence of low porewater sulfate (SO₄²⁻) concentrations under highly reducing (methanogenic) conditions. This supports the occurrence of anaerobic sulfide reoxidation (ASR) through intermediate-valence S forms that replenish porewater SO₄²⁻. The goals were to develop a reactive transport modeling framework with the PFLOTRAN code that incorporates “cryptic” S cycle reactions and to evaluate how these reactions control Fe-S-C processes under variable hydrologic conditions that researchers measure at the site. The team constructed an ASR reaction network based on X-ray absorption spectroscopy and metagenomic analyses. Metagenomic results revealed the presence of microbes corresponding to multiple reactions involving sulfur intermediates, with the highest

functional S gene abundance throughout the vertical soil profile of those capable of anaerobically oxidizing thiosulfate (S₂O₃²⁻). Sulfur XANES confirmed the presence of various intermediate valence S forms. These outcomes prompted incorporation into PFLOTRAN of anaerobic sulfide oxidation to sulfate through thiosulfate and other intermediary sulfur forms, coupled to iron reduction. Monod kinetic reaction rate parameters were manually calibrated to simulate redox activity through thiosulfate pathways as well as to match observed aqueous SO₄²⁻, Fe, and methane concentrations. Preliminary model scenarios show the dominance of ASR under upwelling conditions compared to downwelling for driving Fe-S-C cycling.

Laboratory and Field Studies of the Redox Dynamics of Iron and Uranium in Iron Flocs in Riparian Wetlands Within the Tims Branch Watershed, Savannah River Site

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<https://www.anl.gov/bio/project/subsurface-biogeochemical-research>

The discharge of metallurgical process wastewater containing uranium (U) and co-contaminants (e.g., nickel, chromium, zinc, and lead) from a former nuclear material production facility (i.e., M Area at the Savannah River Site) led to extensive contamination of the downstream wetlands along Tims Branch. Abundant orange and reddish-brown flocs have been repeatedly observed along gaining sections of Tims Branch, where anoxic groundwater containing iron(II) discharges into oxygenated stream water. These flocs contain high levels of iron (Fe; 8–17 wt%, primarily in the form of ferrihydrite and lesser amounts of lepidocrocite and Fe-organic complexes as determined by Fe K-edge extended X-ray absorption fine structure spectroscopy), and are effective scavengers of phosphorus (P; 2–4 wt%), U (32–600 ppm), and trace metals. The flocs initially form under oxic conditions. However, accumulation of flocs can lead to burial of older floc material and the development of anoxic conditions.

Furthermore, during periods of enhanced stream flow (e.g., storm events), accumulated anoxic floc material can

become resuspended in oxic stream water. Thus, biogeochemical processes and attendant changes in redox conditions within the flocs are likely to affect the speciation of redox active constituents (e.g., Fe and U) and, potentially the bioavailability of nutrients such as P. Laboratory microcosm studies of 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), as determined by X-ray absorption fine structure (XAFS) analysis; following a return to oxic conditions, Fe(II) and U(IV) oxidize back to Fe(III) and U(VI). XAFS analysis along the depth profile of accumulated floc material collected in Tims Branch shows

a progressive reduction of Fe(III) to Fe(II) and U(VI) to U(IV) with depth, consistent with the observed decrease in redox potential and analogous to the behavior of Fe and U during redox manipulations in this microcosm study. Given that Fe flocs are frequently observed in a broad range of wetland environments, these studies of Fe floc biogeochemistry in Tims Branch and its potential impact on U speciation and transport expand the scientific community's understanding of Fe floc's role in the speciation and cycling of trace elements in wetlands, which in turn can lead to more robust modeling of trace element behavior in aquatic and terrestrial environments.

IDEAS

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

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ideas-watersheds.github.io

Through its watershed-focused science focus area (SFA) projects, the ESS program is tightly integrating observations, experiments, and modeling to advance a systems-level understanding of watershed function and to translate that understanding into advanced science-based watershed system models. To enhance and broaden the impact of existing SFAs, the IDEAS-Watersheds project strives to increase watershed modeling capacity by increasing software development productivity—a key aspect of overall scientific productivity—through an agile approach to creating a sustainable, reliable software ecosystem with interoperable components.

The unique structure of the IDEAS-Watersheds (Phase 2) project is organized around four research activities and four shared infrastructure activities. To ensure integration of the research activities with the SFAs and to facilitate training of early career researchers, a co-funding model was used with shared deliverables to establish partnerships. The partnerships increasingly embrace a multiscale perspective of the whole watershed and include the Watershed Function SFA (Lawrence Berkeley National Laboratory; LBNL, poster led by S. Molins), the Watershed Dynamics and Evolution SFA (Oak Ridge National Laboratory, poster led by Phong Le), and the River Corridor SFA (Pacific Northwest National Laboratory, poster led by Xingyuan Chen). In addition, a targeted research activity on floodplain hydro-biogechemistry with the Floodplain SFA (SLAC National Accelerator Laboratory) will advance fine-scale reactive transport modeling capabilities (see LBNL poster). 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.

Shared infrastructure activities provide foundational support for 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 easier to use by coordinating software design, development, maintenance, testing, and more accessible deployments. A new Land Model Interface Activity will assess the complex issues around interoperability of land models with integrated hydrology 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, a Training, Community Building, and Outreach Activity will continue building a community around the software ecosystem.

Toward Data-Informed Process-Based Models of Watershed Function

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Aggregate measures of mountainous watershed responses, such as concentration–discharge (C–Q) relationships, are available from point measurements at gauged streams. However, this response is the result of the complex coupling between hydrologic, biogeochemical, and ecological processes across the different watershed subsystems, including hillslopes and floodplains, and across scales. Spatially resolved (or distributed) mechanistic models play an important role in quantitatively understanding and predicting this response. For an accurate system representation, models must consider the gamut of processes affecting energy and mass balances. At the same time, process-rich models must be able to incorporate the heterogeneous datasets derived from field campaigns, as well as geological and machine-learning models, at different scales of observation. In turn, model insights will then be used to inform the need for additional observations in a classical ModEx loop.

This presentation illustrates how to use workflow and simulation tools in the IDEAS-Watersheds software ecosystem to incorporate a variety of datasets and perform simulations of integrated hydrology and reactive transport. Specifically, these tools are applied to the Lower Triangle Region (LTR) use case in partnership with the Watershed Function science focus area (SFA), a headwater-dominated catchment of the

East River, Colorado, that comprises hillslope and floodplain subsystems.

Watershed Workflow is used to mesh the simulation domain with variable resolution following the streams in LTR, and to process datasets of vegetation cover, organic carbon, and subsurface geological materials to assign heterogeneous properties to the mesh at the appropriate resolution. Simulations are performed with the Advanced Terrestrial Simulator (ATS) and constrained by integrated C-Q data both at the upstream and downstream.

At finer scales, floodplain architectures dictate exchange between streams and surrounding groundwater systems. Strong vertical layering of fine-grained sediments over coarse-grained units can create strong redox gradients, where anoxic conditions in fine-grained units exchange with underlying oxic gravel aquifers. The degree of exchange can mobilize colloids and release metals into the stream. Expanded treatments of carbon, iron (Fe), and sulfur redox cycling, with an emphasis on Fe-colloid formation and mobilization, are being developed in partnership with SFA work through the SLAC National Accelerator Laboratory at the Slate River, Colorado. These improved fine-scale process models form the basis upon which process complexity is being expanded in watershed models.

A Multiscale Integrated Hydrology Model for Transport in River Basins

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Solute movement in a watershed is a complex process with multiple interactions and feedbacks across various spatial- and timescales. Understanding how solute moves along diverse hydrologic pathways through watersheds—from hillslopes to channels and in and out of the hyporheic zones—is challenging but critically important since these processes integrate and contribute to the biogeochemical functioning of the river corridor up to the river network scale. In partnership with Oak Ridge National Laboratory's Watershed Dynamics and Evolution science focus area (SFA), the IDEAS-Watersheds project is developing a multiscale integrated modeling framework for transport at the river basin scale. The framework combines a fully integrated surface/subsurface flow model with a multiscale transport model in which the dynamics of transport and reactions in the hyporheic zone adjacent to stream channels are described in Lagrangian form as a subgrid model.

The framework is implemented in the Advanced Terrestrial Simulator model, which provides great flexibility in simulating flow and transport over multiple interacting meshes. It also links to biogeochemical reaction capabilities in the PFLOTRAN code, thus enabling multiscale reactive transport models. Researchers demonstrate multiscale models where flow dynamics are simulated over the entire watershed, but reactive transport is localized to the stream network and associated hyporheic zones. This greatly reduces computational cost without losing the effect of biogeochemical hot spots on downstream water chemistry. The research team first demonstrates the model using the synthetic tilted open book catchment. Then they simulate a long-term network-scale test at the H. J. Andrews Experimental Forest in the western Cascade Mountains, Oregon, and successfully compare it to observations. Model results demonstrate that the proposed framework can link hydro-biogeochemical processes occurring at small scales into a network context to help understand how small-scale processes cascade into network-scale effects, a common scaling challenge across ESS SFAs.

Watershed Hydrologic and Biogeochemical Responses to Wildfires in the Pacific Northwest

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ideas-watersheds.github.io

The IDEAS-Watersheds project focuses on developing general modeling capabilities and workflows that leverage a community software ecosystem to advance hydro-biogeochemical 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 (DOM) chemistry, microbial activity, and disturbances on river corridor hydro-biogeochemical function from watershed to basin scales. Researchers use the Advanced Terrestrial Simulator (ATS) and PFLOTRAN code coupled through the Alquimia interface (ATS-PFLOTRAN) to investigate watershed post-fire hydrologic and biogeochemical responses under various precipitation scenarios across a range of watersheds.

In addition to using MODIS-sensor-informed phenology to capture post-fire vegetation cover changes, a new fire module within ATS-PFLOTRAN was also implemented to account for the water repellency of the surface soil burned at different severities. The top layer soil permeability and hydrophobic layer depths were modified based on mapped burn severity from the Monitoring Trends in Burn Severity database. The model results reveal that wildfires enhance surface runoff and suppress infiltration, with nonlinear relationships with post-fire precipitation events that vary under different combinations of pre-fire land cover types with pre-fire surface soil permeabilities. This modeling framework is poised to account for fire-induced changes in DOM

characteristics by integrating the parallel IDEAS-Watersheds effort in developing pipelines that link organic carbon speciation with biogeochemical models and then with continuum reactive transport models in PFLOTRAN. Narrative examples were shared with the broader community in the Jupyter notebook to encourage adoption of such mechanistic watershed hydro-biogeochemical models in other watersheds and river corridors. 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.

Other National Laboratory-Led Projects

Virtual

Scaling Hydrologic Models from Watersheds to River Basins Using Machine Learning and Coprocessors

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<https://exasheds.org>

Threats to water quality and quantity are of utmost concern as society grapples with a changing Earth system. Dwindling freshwater supplies in arid systems; nitrogen loading in agricultural systems; and pollutants, salinity intrusion, and flooding in coastal urban systems are of crucial importance in a changing climate. While many ESS projects continue to advance process understanding at scales at which those processes can be observed directly and modeled (often at the hillslope or small catchment scales), Earth and environmental system modeling projects face the difficult challenge of integrating process understanding into models at the global scale. To address this challenge, the ExaSheds project has developed and demonstrated a key linking capability that scales process understanding from the site level to full river basins.

The research team describes a model-centric scaling strategy—developed and partially demonstrated in the ExaSheds project—that combines machine learning and process-based simulation to enable high-resolution, process-based simulations of hydro-biogeochemical function at full river basin scales. The Advanced Terrestrial Simulator code (ATS) demonstrates how programming models that abstract the supercomputer's architecture can enable high-resolution process-rich models informed by diverse data products to run on heterogeneous architectures at increasingly large scales. Machine learning is used to represent components of the hydrologic system that have uncertain process representation. For example, machine learning can be used to represent reservoir operations within an ATS model, focusing on the impacts of reservoirs on the river basin water cycle.

Finally, the Gunnison River Basin was used to demonstrate an approach where ML-based surrogate models are trained

on ATS simulations of selected subbasins and then transferred spatially and temporally to predict long-time function of full river basins.

Downscaling of Past and Future Climate Forcing

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An accurate characterization of snowpack water content is necessary to quantify water availability. Lidar technology can quantify snowpack at high resolution scales of ~1m and finer but the frequency of these observations is very low. In this study, scientists developed a machine-learning framework based on random forests, which is capable of estimating snowpack at time points when lidar observations via Airborne Snow Observatories are not available. The framework approximates the physical processes governing accumulation and melt, as well as snowpack physical characteristics. Fifteen different variables were used, derived from precipitation, temperature, surface reflectance, elevation, and canopy. The framework was implemented in the Rocky Mountains of Colorado and the snowpack estimates were found to be more accurate than those of the Snow Data Assimilation System (SNODAS), a respected industry standard. Specifically, the coefficient of determination using the new framework was 0.57, which is a significant improvement from 0.13 obtained using SNODAS. Additionally, the effects of different types of variables for modeling snowpack were investigated by developing three different models. Precipitation and temperature were found to be more important than surface reflectance. This research provides a way to expand the applicability of costly lidar data, which helps to improve snowpack estimation that is critical for water resource management (Mital et al. 2022).

A second effort involves taking future climate data from the Coupled Model Intercomparison Project 6 (CMIP6) to model future global climate using shared socioeconomic pathways (SSPs). Five different SSP scenarios project global warming ranging from 1.4°C (best) to 2.4°C (worst) by the end of the century. Although the CMIP6 model resolution is >100 km with daily time data, higher resolution CMIP6 downscaled datasets do exist, such as the NASA Downscaled CMIP6 dataset with 25-km spatial resolution. However, the integrated surface-subsurface Advanced Terrestrial Simulator (ATS) model requires downscale model outputs <1 km. Using the NASA Downscaled CMIP6 dataset, a

modified U-Net architecture is being developed to learn statistical relationships between coarse resolution (25 km) and fine resolution climate (800 m). Efforts are underway to incorporate these high-resolution climate data into Amanzi-ATS to understand future water availability in the Rocky Mountains of Colorado.

Mital, U., et al. 2022. "Modeling Spatial Distribution of Snow Water Equivalent by Combining Meteorological and Satellite Data with Lidar Maps," *Artificial Intelligence for the Earth Systems* 1(4), e220010.

Early Career

Influence of Drying on Riverine Sediment Biogeochemistry Across the Contiguous United States

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Global change is altering where and when there is enough water for streams to flow. This leads to changes in where and when riverine sediments are inundated with an overlying water column, and it affects the associated wet and dry dynamics those sediments experience. Previous work has shown that these changes in inundation and wet and dry dynamics have strong influences over biogeochemical rates, organic matter chemistry, and organismal ecology. For example, a global study of riverbed sediments showed that respiration rates increased up to 66-fold upon rewetting. There is a knowledge gap regarding how respiration rates in rewetted sediments compare to sediments that are consistently inundated, and also regarding what factors govern the effect size of drying on respiration.

To help address this gap, researchers are conducting a manipulative laboratory experiment using sediments from the shallow hyporheic zone (~5 cm into the riverbed). The sediments are being crowdsourced from across the contiguous U.S. to span a broad range of environmental conditions. The experiment has two treatments: (1) sediments are allowed to air dry; and (2) sediments are kept inundated. In both cases sediments are constantly shaken to encourage aerobic conditions. After three weeks of these conditions, aerated water is added to both treatments to remove all headspace and oxygen (O) consumption is measured over two hours using custom built O optodes that provide data every two minutes. Results show that in some sites drying and rewetting has almost no influence over respiration rates. Yet in other sites, drying and rewetting leads to dramatically

lower respiration rates in air dried sediments compared to rates in consistently inundated sediments. These initial outcomes complement previous work showing that while respiration rates following rewetting may be elevated compared to dry conditions, rates following rewetting may not be elevated compared to rates in consistently inundated sediments. Combining insights from previous work and the current experiment can, therefore, provide an increasingly holistic understanding of the biogeochemical impacts of changes in where and when streams flow.

Early Career

Examining the Impacts of Disturbances on River Hydrology at Regional to Continental Scales

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<https://sites.google.com/lbl.gov/inaiads>

Hydrometeorological disturbances such as floods, droughts, and heatwaves are projected to increase due to climate change impacting river water availability and quality. This presentation examines the effects of disturbances, and particularly drought, on river flow, temperature, and salinity across different watersheds in the United States. An overarching goal is to determine how watersheds with different traits such as climate, topography, vegetation, and land use respond to disturbance. First, the team presents a conceptual framework to study the resistance of hydrologic catchments to droughts and demonstrates its utility by studying the California megadrought (2012 to 2015). Researchers find that human-impacted catchments were more resistant to meteorological drought compared to pristine catchments and that the prolonged drought period and cumulative impact of prior drought episodes impaired catchment resistance. The team then shows how periods of severe drought throughout the last 20 years resulted in annual streamflow decreases and increases in water temperature and specific conductance in the Upper Colorado River Basin. Natural (e.g., average summer rain and forest cover) and anthropogenic (e.g., distance to dams) traits are found to be correlated with the relative change of each variable as well as the variation within sites. Finally, the team presents a novel network-based method for multiscale catchment classification using watershed traits, where the relationships between catchments are represented by the edges of a network. The ability of networks is

leveraged to capture collective behaviors to find clusters of catchments with similar traits at a particular scale. Researchers first build a network of 274 traits and determine a small number of interpretable trait categories based on their similarity. The network method is then applied using the trait categories to classify 9,067 river catchments across the contiguous United States. The resulting classification shows a remarkable geographical coherence across traits categories. Additionally, the team finds that different catchment clusters have distinct hydrologic behavior (e.g., streamflow statistics). This approach allows the establishment of a connection between catchment hydrological behavior, including their response to disturbance and physical traits.

Small Business Innovation Research / Small Business Technology Transfer Research

Rhizomatic: Next-Generation Image Processing for *In Situ* Fine Root Measurement

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Oceanit Laboratories have developed “Rhizomatic,” an automatic root analysis and characterization tool to help plant scientists better understand the “hidden half” of plant systems and produce research more quickly, more reliably, and more reproducibly. Rhizomatic has been developed as a web application to which users can upload images of *in situ* root systems taken by minirhizotrons or other imaging methods and either use existing prediction models to automatically find and characterize the roots present or, without a background in machine learning, easily train their own models customized to the specifics of their root study. Predicted roots are tracked over time across multiple sessions and growth and topology can be automatically measured and tracked.

Unlike other root prediction software, Rhizomatic only requires the standard, line-based root marking commonly performed in minirhizotron root tracing projects to train new models, enabling the development of models without new root tracing. Rhizomatic is currently compatible with Rootfly, RootSnap, rhizoTrak, and WinRHIZO Tron programs; marking software and other root tracing formats can be added easily. Additionally, as the model library grows, users will be able to reliably find pre-trained prediction models shared by other scientists, both reducing the need for human-traced roots and providing a tracing solution that will produce tracings and metrics that can be directly compared to each other without the concern that different root tracers have different standards. Collection of a body of ever-improving models is expected over time.

In addition to the automatic root prediction core, Rhizomatic includes an image processing pipeline that can address and fix common errors in root imaging. It can screen out bad images if they are significantly dissimilar to others from the same window, repair severely misaligned and mislabeled images by finding their correct window, and adjust root marks copied from a previous image and not updated to compensate for imager misalignment. Finally, as many prior studies may have incomplete tracings that may not produce the best prediction models, Rhizomatic’s root review tool can be used to review predicted roots against prior tracings, approve correct predictions, and then retrain with updated tracings to bootstrap into a higher quality root prediction model.

COASTAL SYSTEMS

University Projects

Functional-Type Modeling Approach and Data-Driven Parameterization of Methane Emissions in Wetlands

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The role of natural wetland emissions in the recent sharp increase of global atmospheric methane concentrations is hotly debated. Difficulties in modeling methane emissions are driven, in part, by the spatially heterogeneous nature of wetland ecosystems. This variability in fluxes is a result of the underlying within-wetland heterogeneity, combined with the complex and interconnected below- and above-ground processes of methane production, consumption, and transport. The goal of this project is to improve the simulation of methane emissions from coastal wetlands using E3SM Land Model (ELM). Researchers will improve ELM along three spatial and conceptual axes: (1) patch resolution: expand the sub-grid surface-tile approach to represent ecohydrological wetland patch types, such as open-water, mudflats, floating vegetation, cattail marsh, swamp forest; (2) vertical resolution: provide detailed observations of belowground dissolved methane concentration gradients and utilize ELM's patch-level vertical soil column to resolve methane production, oxidation, and transport at high vertical resolution per patch; and (3) process resolution: provide observations of process-specific parameters that will be used to improve the resolution of processes within the complex system that drive net methane fluxes.

The team has completed the development of a revised version of the methane module in ELM. The new version resolves wetlands as a land unit with the ability to resolve multiple different eco-hydrological patches within a wetland. The team allowed prescribing maximal inundation depth as a forcing. Researchers prescribed patch area distribution from classified remote sensing images. The team developed the Bayesian Optimization for Anything (BOA) package and wrapped ELM with this optimization engine. Researchers used eddy covariance observations of carbon fluxes to parameterize photosynthesis, respiration, and methane production. They prescribed observed plant aerenchyma

conductivity to methane and oxygen transport and used vertical profiles of methane concentration in the soil along with chamber flux measurements to parameterize methane production. The team conducted simulations of two sites in Louisiana (US-LA2, US-LA3) where they conducted observations over at least 2 years, running with two to four patch types in each site. The revised ELM model is capable of matching carbon and methane fluxes and soil concentration profiles more accurately than previous models.

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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The 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 2022, researchers successfully established the sampling site (AmeriFlux site US-PLo) in a brackish marsh in the Parker River estuary, MA. In addition to the flux tower installation, two sampling locations (marsh interior, creek bank) were equipped with automated sensors (soil temperature, water level, salinity, redox profile) to contrast different soil and hydrological conditions. Researchers also did an initial field test with the new spatially explicit sediment redox measurements. The measurements captured the system response to an extreme drought, which caused high salinity levels (20ppt) early in the growing season.

Researchers will use these field measurements to help constrain three phases of ELM-PFLOTRAN development designed to improve simulations of brackish marsh biogeochemistry under fluctuating oxygen availability and salinity

influenced by tides, diel and seasonal changes in plant physiology and river discharge. Researchers have already implemented aerenchyma-mediated oxygen transport into PFLOTTRAN using data from the sites. Using a simplified reaction network, researchers find impacts on belowground biogeochemical cycling due to the heterogeneous distribution of oxygen in the soil.

Ultimately, researchers will be poised to combine the new process understanding and model formulation with existing long-term data already in hand from two more saline salt marsh sites in the Parker Estuary.

Dynamic Hydrology Shapes Microbial Activity and Biogeochemistry in a Great Lakes Coastal Estuary

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The propensity for redox processes to occur is sometimes predicted by measured or assumed redox potential (E_h), but process measurements often deviate from predictions based on the thermodynamic “redox tower” paradigm. Researchers hypothesize that poorly measured, granular scale soil heterogeneity causes apparent departures from thermodynamic exclusion principles at bulk scales with consequences for biogeochemical cycling, which are not currently resolved in ecosystem, regional, or global scale models. Researchers will combine empirically measured traditional biogeochemical indicators with newly developed electrochemical approaches to determine how fluctuating hydrology shapes redox regimes and processes. Specifically, the objectives are to: (1) relate dynamic hydrology in a freshwater terrestrial-aquatic interface wetland (Old Woman Creek, OH) to redox regimes; (2) determine how redox heterogeneity drives elemental cycling at multiple scales, and; (3) assess the sensitivity of process-based models to the inclusion of fine-scale variability in redox conditions. Researchers will use zero resistance ammetry (ZRA) to exploit redox disequilibria among discrete zones to detect the distributions, extents, and kinetics of biogeochemical processes. ZRA can measure electrical current that arises

from microbially induced redox disequilibrium. In 2021 to 2022, researchers worked to refine a ZRA sensor system that detects electrochemical signals across the sediment-water interface and into sediments at nested scales (sub-millimeter to decimeter) at a shallow location (< 10 cm surface water) in the Old Woman Creek wetland. The team deployed the manufactured sensor system from late June through November in 2022. During that time, the sensors experienced fluctuating hydrologic conditions with depths ranging from zero (no standing water) to at least 50 cm. ZRA sensors detected redox disequilibria, and thus heterogeneous redox conditions, over spatial scales as small as 2 mm.

Concurrent measurements of greenhouse gas fluxes measured in vegetated and unvegetated plots using static chambers in the vicinity indicated that ecosystem functions also responded to fluctuating hydrology. In 2023, the ZRA sensors will be re-deployed in multiple locations simultaneously with traditional redox potential (E_h) electrode sensors. The team will monitor concentrations of redox process substrates and products in surface water, pore water, and sediment samples to relate electrochemical signals to biogeochemical processes. To assess the importance of fine-scale heterogeneity in ecosystem-scale processes, researchers are incorporating microsite heterogeneity into the *ecosys* ecosystem model.

Experimental Research on Environmental Fate and Transport Processes in Support of University of Houston/Pacific Northwest National Laboratory Partnerships

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This Research Development and Partnership Pilot (RDPP) project focuses on establishing research connections between the Pacific Northwest National Laboratory (PNNL) and the University of Houston (UH; including PIs from Civil and Environmental Engineering and Biology and Biochemistry). The partnership broadly explores potential research directions related to coastal systems, including: (1) development of Earth system models; (2) application of remote sensing methods, and; (3) experimental research in coastal wetlands. This presentation will specifically focus on the experimental research components, including laboratory-based research to investigate the environmental fate and transport behavior of colloids and their interactions with natural organic matter. Research products from this

project component include the development of new analytical methods for advanced characterization of colloids, emerging contaminants such as microplastics, and their co-contaminant transport behavior, as well as fundamental modeling of colloidal stability, deposition, and reactivity. In addition, the research capabilities available at a new experimental wetlands facility at the UH Coastal Center will be presented. This facility will enable controlled and replicated experimentation on biogeochemical processes under varied conditions (i.e., flooding or salinity intrusions) at a mesocosm scale. Opportunities for collaboration between UH, PNNL, and other DOE ESS laboratories to support broader research on sediment and contaminant fate in coastal systems will be discussed.

Virtual

Exploring the Influence of Dual Stresses of High Salinity and High Vapor Pressure Deficits on Water Transport in Mangroves

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

Here, researchers present results of a combined greenhouse and field study of responses of the mangrove species *Avicennia germinans*, *Avicennia marina*, and *Rhizophora mangle* to fluctuating humidity and salinity conditions. Water uptake in plants is limited by both water supply within the root zone and water demand by the atmosphere at the leaves. For most mangroves, water availability to roots is limited not by the presence of water, but by salinity concentration and the time and energy necessary for the development of the osmotic potential gradient, which drives water uptake. Researchers studied sap flux, stem and leaf water potential,

stem hydraulic conductivity, stomatal conductance, and net photosynthetic assimilation of carbon for each of the three species in order to assess responses to high vapor pressure deficits and high salinities. Observations were also used to create species-specific plant hydraulics parameters for use with the FETCH plant hydrodynamics model, which researchers have augmented to mechanistically include osmoregulation of water uptake by halophytes. FETCH-osmo is designed to promote analysis of mangrove forest function across both humidity and salinity gradients, which are predicted to change in response to disturbances such as sea level rise, precipitation variability, inundation frequency, and increased atmospheric carbon dioxide. Ultimately, the new FETCH-osmo model will be integrated into the DOE's functionally assembled terrestrial simulator (FATES) within E3SM.

Plant-Microbe Feedbacks Drive Coastal Wetland Responses to Global Change

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Warming temperatures and elevated carbon dioxide (CO₂) may increase wetland productivity and organic matter accumulation, but unknown plant-microbe feedbacks make it difficult to model how wetlands will respond to global change. The Salt Marsh Accretion Response to Temperature eXperiment (SMARTX) was established in the Smithsonian's Global Change Research Wetland in 2016 to advance model representation of coastal wetland responses to global climate change. In SMARTX, researchers actively manipulate whole-ecosystem temperature through feedback-controlled heating from the plant canopy to 1.5 m soil depth, as well as atmospheric CO₂ concentration.

Throughout the experiment, a moderate amount of warming (+1.7 °C) has consistently maximized marsh elevation gain and belowground carbon (C) accumulation, consistent with previously observed nonlinear effects on belowground net primary productivity (NPP), which researchers hypothesized was driven by asynchrony between the microbially mediated supply and plant demand of nitrogen (N). Using a classic “functional balance” model depicting root vs. shoot allocation, researchers have recently been able to accurately predict annual belowground NPP as a function of plant N demand and soil N supply. This work provides the first model of marsh C accumulation that treats root-to-shoot

ratios as dynamic, capturing the coupling of N-cycling and C storage.

At higher temperatures, marsh elevation loss increased and was associated with increased C mineralization and micro-topographic heterogeneity, a potential early warning sign of marsh drowning. Under warming conditions, the balance between microbial decomposition and NPP is largely negative, with high rates of decomposition (inferred from methane emissions) reducing organic matter storage. This likely interacts with plant effects, where high root growth during the summer brings in oxygen and organic C, increasing rates of decomposition. Elevated CO₂ also led to a decline in C accumulation, especially when combined with warming, despite increased inputs of belowground NPP. This indicates that enhanced root production under future climate conditions may not increase marsh resilience, due to plant-microbe feedbacks resulting in high rates of aerobic decomposition.

Combining Hybridization Chain Reaction–Fluorescence *In Situ* Hybridization and Multiplexing to Map Salt Marsh Sediments Microbial Community

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Salt marshes are among the most biogeochemically active environments on Earth. They display an important microbial diversity due to high organic matter input, active tidal cycling, and vegetative colonization. Sequencing technologies have expanded the ability to analyze the microbial population of such complex environments. While it is possible to answer the question of diversity composition, sequencing analysis does not allow researchers to discern the interactions within the microbial community and between the microorganisms and their environment. To this extent, the method of fluorescence *in situ* hybridization (FISH) is a powerful tool, allowing us, via specific hybridizations, to not only have a visual confirmation of sample diversity, but to observe how the microorganisms are interacting with each other, like symbiosis or predator–prey relationships. Unfortunately, salt marsh sediment poses some technical challenges with the most important being the sediments autofluorescence, making microorganism identification challenging. Furthermore, the intensity of the signal depends on the individual activity of microorganisms. This activity can be low in sediments, and therefore, it can be challenging to observe and differentiate microorganisms within the matrix. Hybridization chain reaction (HCR) FISH is a recently developed

technique that allows researchers to observe such diversity with a strong signal while getting over the autofluorescence emitted by the sample matrix by increasing the contrast between labeled microbes and matrix grains. This method is based on the hybridization of initiator probes, targeting a sequence of interest. The presence of initiator probes triggers hybridization with two supplementary labeled probes called amplifiers. The resulting effect increases the signal, causing a higher contrast between the targeted organisms and the matrix. Here, for the first time, researchers used HCR-FISH to identify microorganisms composing the Little Sippewissett microbiome and how they interact within the sediments. The team developed a multilabeling method to efficiently target organisms' housekeeping genes to identify specific key players in the salt marsh geochemical cycle. The resulting color code allows the team to not only precisely identify microorganisms but shows the interactions between each of them. From those observations, researchers can evaluate the dominance of certain key players in the sediment and how they influence the biogeochemical cycle of salt marsh sediments. This new application of HCR-FISH could be a template for further study based in sediments and could be extended to fill in the gaps between microbial diversity and microbe interactions with its environment.

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 systems are the strongest long-term carbon (C) sinks per unit area, yet these ecosystems, and the biogeochemical processes regulating C exchange, are not well represented in Earth system models. In 2021, NATURA (A Network of North American Tidal Wetlands: Understanding Through Coordinated Research Activities) was established, funded by DOE. This project unites seven eddy covariance flux sites along the east and west coasts of the United States and Canada and aims to

improve empirical understanding and assist process-based biogeochemical modeling of these critical ecosystems. The team coupled field measurements, statistical analyses, and experimental mesocosms in a ModEx approach to: (1) improve net ecosystem exchange (NEE) partitioning into gross primary production (GPP) and ecosystem respiration (RECO); (2) quantify the influence of elevation, nitrate, and salinity on GPP and methane fluxes; (3) derive thresholds and responses of C fluxes to nonperiodic pulses of salinity and nitrogen; and (4) inform and improve biogeochemical models, MEM-PEPRMT and PFLOTRAN-E3SM. Analysis of three NEE partitioning approaches revealed high variability in performance both within and across tidal wetlands ($n=6$ eddy covariance sites). This variability likely resulted from pulses of nitrate and salinity as well as tidal pumping of dissolved carbon dioxide and other forms of respired C. Stable isotope partitioning and lateral C flux measurements were used to evaluate and improve partitioning algorithms. Researchers improved MEM-PEPRMT model performance across sites by incorporating nitrate and salinity data from the tidal channel to help predict GPP, RECO, and methane exchange. The team is now in the process of standardizing nitrogen, salinity, water level, and additional measurements in all seven NATURA sites and, in spring 2023, will begin running mesocosm experiments using a ModEx approach to isolate the effects of nitrogen and salinity on GPP and methane fluxes.

Early Career

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

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Greenhouse gas production and fluxes in coastal wetlands are controlled by complex interacting hydrological and ecological processes whose dynamics are, in turn, modified by saltwater intrusion (SWI) events. In suburban and urban transition zones of many coastal areas, the floodwalls and levee systems built to protect infrastructure and urban development intensify the SWI events resulting from floods during storm surges. When the flood waves travel inland, they meet these barriers, and saltwater can remain stagnant for prolonged periods, increasing the exposure of adjacent coastal wetlands to salt stress (i.e., persistent SWI events). These stress conditions induced by SWI are rarely represented in biogeochemical models, limiting the capacity to predict and assess the long-term effects of SWI on coastal greenhouse gas production and fluxes. Moreover, significant

knowledge gaps exist in how the ecosystem reorganizes after SWI disturbance.

Specifically, what trajectories do biological components (ecosystem structure), greenhouse gas production, and emission (ecosystem function) follow after SWI? Also, it is not clear what the relevant scales are for evaluating these trajectories. Using an ecohydrological patch approach defined by plant functional types and water levels, this early career proposal aims to better understand how ecosystem structure and function linked to greenhouse gas fluxes in freshwater coastal wetlands affected by the built environment are influenced by SWI in the short- (days to weeks) and long- (years to decades) term. This project evaluates carbon dioxide (CO_2) and methane (CH_4) pools and fluxes before, during, and after simulated SWI events covering a wide range of salt exposure (salinity concentration, duration, and frequency).

The measurements will be conducted with a multisetting sampling approach composed of controlled mesocosm in greenhouses and experimental wetland ecosystem units. It will be complemented with time-for-space replacements in coastal wetlands with a history of persistent SWI. Data collected will be used to produce and incorporate an explicit salinity-dependent function into the CH_4 biogeochemistry module integrated into the E3SM Land Model (ELM v1). Early testing on experimental wetland ecosystem units with simulated SWI events of ~ 2 psu salinity concentrations and durations of one, three, and five days indicate that CO_2 and CH_4 fluxes were affected after five days in cattail and maidencaine patches. CH_4 fluxes in maidencaine patches were also affected by SWI events of three days.

The Push and Pull at the Land–Sea Interface: How Bidirectional Freshwater and Marine Inputs Drive Hydro-Biogeochemical Function in Salt Marsh Sediments

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<http://mzimmer.weebly.com/nitrates.html>

Salt marshes exist at the terrestrial–aquatic interface between watersheds and adjacent marine environments. These systems receive hydrologic inputs at a range of time

scales, from daily tidal cycles to seasonally elevated groundwater. These bidirectional water sources can cause rapid as well as seasonal changes in a range of environmental conditions in marsh sediments, including saturation, salinity, and redox conditions. However, there is limited understanding of how these time-variable environmental conditions drive the hot moments, or temporal dynamics of nutrient processing, within marshes. To address this knowledge gap, researchers instrumented a 25 m transect along a representative salt marsh platform at the Elkhorn Slough National Estuarine Research Reserve in California. The team installed variable-depth redox probes, nested piezometers, and a field-deployable spectrophotometer at lower, mid, and upper marsh positions to allow for characterization of subsurface hydrologic cycling and biogeochemical behavior

at a high frequency. Researchers also conducted seasonal sediment incubation experiments to quantify nitrogen processing rates as well as monthly vegetation surveys, monthly pore water sampling campaigns, and subsurface sediment characterization. The team found that biogeochemical behavior ranged as a function of time scale. Findings suggest that intra-annual changes in source water contributions across the marsh result in functional zonation, where lower marsh position functions may be regulated by tidal flushing and upper marsh position functions may be regulated by freshwater contributions. A reactive transport model is being developed to extend process understanding into additional scenarios that investigate how changing hydrologic conditions (e.g., sea level rise, precipitation extremes) may affect marsh sediment biogeochemistry.

Science Focus Area

Student

How Does Prolonged Flooding Alter Microbial Carbon and Nutrient Demands Across Coastal Terrestrial–Aquatic Interfaces in the Great Lakes?

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<https://compass.pnnl.gov/FME/COMPASSFME>

Although soil microbes respond rapidly to environmental stimuli, it is unclear how flooding affects carbon (C) availability and turnover rates in coastal ecosystems of the Great Lakes region. As part of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales–Field, Measurements, and Experiments (COMPASS-FME) pilot project, this study aims to disentangle the effects of prolonged flooding on soil microbes and their mechanisms for adaptation. Generally, C availability and turnover rates are limited by extracellular enzyme activity and nutrient availability; however, dominant controls are expected to shift from nutrient to oxygen limitations under hypoxic conditions. Moreover, the team predicts oxygen limitations will reduce dissolved organic carbon (DOC) availability and microbially derived nutrients by inhibiting enzyme activities. To test this hypothesis, researchers conducted a microcosm experiment on soils from three zones across a terrestrial–aquatic interface (TAI) at Old Woman Creek, OH. This site spans an upland deciduous forest, a water-stressed deciduous forest transition, and an inundated wetland. Soils were subjected to nonflooded (oxic) and flooded (hypoxic) treatments and destructively harvested on days 0, 7, 21, and 55 to determine C turnover via C mineralization, potential rates of microbial C and C, nitrogen (N), and phosphorus (P) acquiring enzyme activities, and extractable C, N, and P pools. Results showed oxygen limitations immediately decreased C turnover and DOC in upland and wetland soils ($p < 0.05$) but not in transition soils. Interestingly, C mineralization increased episodically in both flooded wetland and transition soils, corresponding to declines in microbial C and increased DOC and nitrate; however, this DOC was quickly mineralized in flooded wetland soils but not in flooded transition soils. Enzyme stoichiometric analysis revealed that polymeric carbon catalysis remained constant regardless

of TAI location or treatment, indicating that slow exoenzymes turnover provided a lag in biogeochemical responses. Overall, these results suggest a shift from nutrient to oxygen limitations occurs within days across the TAI in response to flooding, but increased microbial turnover is responsible for episodic increases of DOC, nutrient availability, and C turnover. Therefore, further research is required to determine the effects of hypoxia on microbial communities and the accessibility of soil C sources of varying chemical quality to better predict how microbial responses to flooding affect C and nutrient cycling across TAIs.

Understanding the Mechanisms of Conifer Tree Mortality from Seawater Exposure Using E3SM Learning Model (FATES-Hydro)

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Widespread tree mortality in coastal regions associated with sea level rise has been observed globally. Rising sea level is threatens coastal forests through rising porewater hypoxia and salinity. Although the physiological effects of hypoxia and salinity has been well studied, few studies have tested these mechanisms under conditions of coastal tree mortality.

Likewise, there has been very limited model development for simulations of coastal woody-plant mortality. In this study, researchers incorporate the effect of porewater hypoxia and salinity on plant physiology in an ecosystem demography model that incorporates plant hydro-dynamic processes (FATES-Hydro) to investigate the loss of conifer trees from sea water exposure.

The major model developments included: (1) osmotic reduction in soil water potential due to salinity; (2) root death and reduction in belowground conductance due to

hypoxia and salinity; (3) osmotic impact on xylem water potential and conductance; and (4) photosynthetic capacity loss from reduced biochemical reaction rates.

The team conducted numerical experiments at three coastal conifer forests. One is a spruce forest in the Pacific Northwest at Beaver Creek (BC) that has experienced a dramatic increase in tidal seawater exposure since 2015 when a culvert was removed. The other two are loblolly pine forests on the Chesapeake Bay (CP) on the western shores that have experienced gradually increasing sea water exposure from sea level rise. All sites experienced significant tree mortality by 2019. The team conducted a 10-year simulation at BC (2010 to 2019) and a 30-year simulation at CP (1990 to 2019).

The conifer species at the coastal areas have safe and sensitive stomata. With gentle and slow increase of salinity (less flood) at CP, this strategy leads to less hydraulic stress, negative carbon (C) balance, and mortality is mainly caused by C starvation. The sudden and dramatic rise of soil salinity and hypoxia at BC, in contrast, causes a significant drop of soil water potential and a quick loss of xylem conductivity resulting in significant hydraulic stress. Hydraulic failure is the main cause of mortality; over time the hydraulic stress reinforces the negative C balance and promotes C starvation driven mortality. This analysis benchmarks model performance while providing testable hypotheses for future experiments.

Soil Saturation Response to Changing Hydrological Regimes at Coastal Interfaces

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Coastal interfaces are increasingly experiencing changes in their hydrological regimes with more dynamic wetting and drying frequency and duration caused by increased storm surges, flooding events, lake level fluctuations, and sea level rise. This results in high temporal and spatial variation in soil saturation, which impacts ecological functions from plant growth to biogeochemical cycling. Improved measurements and models are required to capture varying soil-water saturation dynamics and quantify changes in storage. This study aimed to delineate soil stratigraphic connectivity and capture hydraulic state changes during

hydrological perturbations across the coastal interface using geophysical models validated with *in situ* soil cores and hydraulic parameter measurements. The team also developed a hydro-geophysical framework combining geophysics and an advanced terrestrial simulator (ATS) flow model to capture the variation in soil saturation at coastal interfaces. Researchers combined electrical resistivity and ground penetrating radar to estimate lateral and vertical variation in soil hydro-stratigraphic properties. A sand-silt-clay stratigraphy characterized the Chesapeake Bay area with a silty clay unit at 1.5 m depth, constraining vertical flow. In contrast, shallow occurrences of glacial till along with silty clays limit vertical flow along the Lake Erie coastal soils. Furthermore, the team used time-lapse electrical resistivity imaging to monitor changes in soil water and solute content during a simulated flooding experiment at a coastal upland forest along the Chesapeake Bay. Resistivity changes of 50% to 85% were attributed to changes in water and solute content revealing fresh and estuarine water infiltration fronts. The flow simulation from ATS captures both saturation and concentration curves extracted from soil sensors and the timelapse geophysical imaging. This study shows the efficacy of using geophysical methods in monitoring hydrological state changes at an ecosystem-scale. The high spatial resolution of geophysical measurements, when converted to hydrological variables, also provides data to calibrate the ATS models. Future work will focus on hydrological investigations coupled with biogeochemical data to mechanistically understand how soil and groundwater dynamics control fluxes and transformations of carbon, nutrients, and greenhouse gasses across coastal-terrestrial-aquatic interfaces.

Geosphere-to-the-Atmosphere: A System Level Analysis of the Immediate Impacts of 10-Year Freshwater and Estuarine-Water Storm Events on a Coastal Forest

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Coastal upland forests are facing widespread mortality as sea-level rise accelerates and precipitation and storm

regimes change. The loss of coastal forests has significant implications for the coastal carbon (C) cycle; yet, predicting the likelihood of mortality is difficult due to the limited understanding of disturbance impacts on coastal forests. The manipulative, ecosystem-scale terrestrial ecosystem manipulation to probe the effects of storm treatments (TEMPEST) experiment is designed to address the potential for extreme freshwater and estuarine-water disturbance events to alter tree function, species composition, and ecosystem processes in a deciduous coastal forest in Maryland. The experiment uses a large-unit (2,000 m²), unreplicated experimental design with three 50 m x 40 m plots serving as control, freshwater, and estuarine-water treatments.

The TEMPEST experiment was successfully launched in June 2022 when researchers completed the first paired storm simulations by delivering 300 m³ of estuarine water (~8 psu salinity) from the mouth of the adjacent Rhode River estuary and commercially sourced freshwater into respective treatment plots using a spatially distributed irrigation network. The water delivery approach saturated the entire rooting zone of the forest (0 to 30 cm) for ~10 hours and elevated the water table by 3 m, producing extensive, low-level (≤ 8 cm above ground) inundation across treatment plots. This single TEMPEST simulation approximated a 13 cm rainfall and based on historic records, was of comparable intensity to a 10-year storm for the area. Here, researchers provide a synthesis of the effects of TEMPEST simulations on the physicochemical (e.g., volumetric water content, electrical conductivity, dissolved oxygen), biogeochemical (e.g., dissolved organic C and nitrogen, soil and tree greenhouse gas fluxes), and physiological (e.g., root respiration, leaf water potential, and sap flow) components of a coastal forest and their comparative resistance and resilience to inundation- and salinity-driven disturbances.

Pairing Field Measurements with Stable Isotope Pool Dilution Shows Acclimation of Gross and Net Methane Fluxes from 4-Year-Old Transplanted Soil Monoliths

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Rising waters in response to global change are shifting coastal terrestrial-aquatic interfaces (TAIs) into previously upland, freshwater-dominated ecosystems. This may result in coastal forest soils transitioning from an atmospheric methane (CH₄) sink to a source, but the sources, timing, and magnitude of such shifts are poorly understood. To disentangle the role of biotic and abiotic factors in soil CH₄ fluxes at coastal TAIs, researchers transplanted soil monoliths from upland to wetland-edge locations (and vice versa) and measured their characteristics and greenhouse gas fluxes over four years. To delve deeper into the microbial processes driving net fluxes measured at the soil surface, researchers used a ¹³CH₄ pool dilution technique to quantify gross methanogenesis and methanotrophy in both transplanted and local soils. The team found that field-net and laboratory-gross rates in transplanted soils were similar in magnitude, regardless of soil origin. The acclimation-to-local conditions indicate low resistivity of CH₄ flux to changes in abiotic conditions. However, gross fluxes from surface soils poorly tracked net fluxes from the integrated soil column. The results demonstrate that soil CH₄ production may rapidly increase in response to increased inundation with estuarine water, and that this flux is more responsive across column depth than increases in CH₄ consumption. Future work will focus on (1) measuring gross rates across depth; (2) determining the relative importance of key features of TAIs, saturation and redox sensitive chemical species; (3) attributing methanogenic (e.g., acetoclastic, hydro-genotrophic) and methanotrophic (oxidation vs anaerobic) processes to measured gross fluxes and their respective taxonomic members; and (4) quantifying how these relationships vary across the broader range of TAI sites that are part of the Coastal

Observations, Mechanisms, and Predictions Across Systems and Scales—Field, Measurements, and Experiments project.

Biogeochemistry of Soils, Sediments, and Surface Waters Across the Upland-to-Wetland Gradient of Coastal Interfaces: Results from the EXCHANGE Consortium

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Coastal terrestrial-aquatic interfaces (TAIs) are hydrologically and biogeochemically dynamic, creating functional gradients that vary substantially over space and time. Cohesive datasets across geographically distributed sites enable an understanding of coastal ecosystem biogeochemical control points and support the transferability of new process knowledge. To achieve a broad and coordinated sampling effort, researchers convened the EXploration of Coastal Hydro-biogeochemistry Across a Network of Gradients and Experiments (EXCHANGE) consortium, as part of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales—Field, Measurements, and Experiments project.

This consortium is a network of researchers that collaborate on the design, methodology, and collection of samples from TAIs in the Great Lakes and Mid-Atlantic regions (Chesapeake and Delaware Bays) of the continental United States. In the Fall of 2021, the EXCHANGE Consortium collected samples from 52 coastal TAIs spanning upland, transition, and wetland soils as well as adjacent surface waters to assess the baseline spatial heterogeneity in chemical forms and distribution of carbon (C), nutrients, and redox-sensitive elements. Researchers found significant differences in physicochemical properties across the coastal TAI regardless of region, while variability in water quality

and nutrient concentrations in the surface waters were regionally dependent. The data shows that while the concentrations of water-extractable organic C were not statistically different, the optical properties of extracted dissolved organic matter (DOM) varied between upland to wetland sample locations, irrespective of region. The corresponding DOM composition in nearby surface waters was distinct from that of soil-extracted DOM from all gradient locations. Oxygen consumption and greenhouse gas concentration patterns during short-term seawater inundation experiments are explained by local soil physical and chemical properties and landscape-scale gradients in salinity exposure. The preliminary results suggest that the region (Great Lakes or Mid-Atlantic) is most important for understanding heterogeneity in surface water biogeochemical parameters, while the position across the upland-to-wetland gradient largely characterizes the variability in soil biogeochemistry. These results are important to validate the range in input parameters of biogeochemical models at transect and regional scales, aiding in the predictive understanding of coastal biogeochemical function.

Time to Anoxia: Oxygen Consumption in Soils Varies Across a Coastal Gradient

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The coastal terrestrial-aquatic interface (TAI) is a highly dynamic system characterized by strong physical, chemical, and biological gradients. Shifting redox conditions due to variations in soil saturation and dissolved oxygen (O) concentrations strongly drive carbon (C) availability and transformations at the TAI. However, it remains challenging to predict across the TAI the rate at which saturation drives aerobic to anoxic shifts in soils with different characteristics and inundation regimes. The research team hypothesized that biological and chemical differences in soils would result in variable O consumption rates across the TAI gradient from uplands to wetlands. To test this hypothesis, researchers integrated field measurements, laboratory incubations,

and model simulations to mechanistically understand O consumption dynamics in coastal soils.

To measure O consumption rates in TAI soils, researchers conducted a laboratory incubation using surface and subsurface soils from a coastal TAI gradient (upland forest to transitional forest to wetland) in the Western Lake Erie region. The cores were inundated with water and incubated for two weeks. Dissolved O concentration was measured continuously over the two-week incubation period using an O-sensitive optode spray.

Wetland soils turned anoxic the fastest, in under 10 hours, whereas upland soils turned anoxic in 18 hours. Upland B-horizon soils did not turn anoxic even after two weeks of saturation in the laboratory, and the O consumption patterns suggest C and/or nutrient limitation in these subsurface soils. These experimental results are consistent with *in situ* redox and O measurements in the field where wetland soils exhibited the highest O consumption rates along the coastal transect. O-D reaction scale simulations with Aquamend accurately captured O drawdown dynamics in these systems. Sensitivity analysis indicated that microbial activity was a strong driver of O consumption in these soils, with the availability of dissolved C fueling microbial metabolism as the key limiting factor of O consumption.

This research, part of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales—Field, Measurements, and Experiments project, provides key context for the understanding of coupled hydrological and biogeochemical processes and contributes to an enhanced understanding of redox controls on C and nutrient cycling across the coastal TAI.

Spatial Variability of Ecosystem Function at Coastal Western Lake Erie

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Recent intensification of the hydrological cycle leads to complex impacts on the functioning of coastal terrestrial-aquatic interfaces (TAIs). Predicting how more intense water level fluctuations alter coastal forest functioning, groundwater and soil redox potential, and greenhouse gas fluxes remains challenging due to the dynamic nature of soil saturation at the TAI. Researchers hypothesized that ecosystem structure of the TAI, defined by depth and duration of soil saturation, drives gradients of (1) groundwater and soil oxygen availability and redox potential; (2) greenhouse gas fluxes from soil and trees with carbon dioxide (CO₂) increasing and methane (CH₄) decreasing from the wetland to the upland; and (3) trees' hydraulic function and photosynthetic capacity, all of which are inversely related to groundwater level below the surface. To measure those changes, researchers are monitoring upland forest-wetland transects at three sites on the southern shore of Lake Erie. The team measured (1) soil and groundwater redox potential; (2) CO₂ and CH₄ fluxes from soil and trees; and (3) tree sap flux. The research team found high variability of redox potential in soil across the TAI, and groundwater redox potential decreased as the groundwater level decreased below the surface, potentially due to decreasing influence of topsoil on inputs of electron acceptors in groundwater. Soil CO₂ fluxes varied spatially, with higher fluxes in wetlands and transition zones than upland areas of

Portage River, possibly due to dry conditions exposing wetland soils or higher organic matter input and root respiration from aquatic macrophytes or flood-stressed trees. Wetlands were the highest sources of soil CH₄ at all sites. The upland zone was a higher sink for soil CH₄ than transition and transitions were a higher source of tree stem CH₄ compared to the upland at two of three sites. Furthermore, flooding of upland forests is associated with a loss of tree hydraulic function, which might reduce canopy, photosynthesis, and carbohydrate storage. This research is part of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales—Field, Measurements, and Experiments project, providing insights into the dynamic relationships between soil saturation and plant and biogeochemical functions regulating the high spatial-temporal variability of TAIs essential for improving the predictive responses to climate change.

Iron Redox Biogeochemistry Across Coastal Terrestrial-Aquatic Interfaces: Field Study in the Great Lakes and Chesapeake Bay Regions

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Coastal terrestrial-aquatic interfaces (TAIs) are highly dynamic environments with spatial and seasonal hydrological fluctuations that impact the geochemical behavior of redox sensitive elements such as iron (Fe) and sulfur, as well as the biogeochemical cycling of carbon and nutrients. The Coastal Observations, Mechanisms, and Predictions Across Systems and Scales—Field, Measurements, and Experiments (COMPASS-FME) pilot study aims to better understand the mechanisms that control the structure, function, and evolution of ecosystem across the coastal TAI. As part of this project, this study aims to better understand Fe redox biogeochemistry across coastal sites in the Great Lakes and the Mid-Atlantic regions of the United States, chosen as model systems to represent freshwater and saltwater coastal environments, respectively. Using X-Ray absorption spectroscopy (XAS), the oxidation state and molecular environment of Fe was determined with depth in undisturbed soil

cores collected across upland to shoreline gradients from coastal locations along the Western Lake Erie Basin and the Chesapeake Bay. XAS results show that Fe occurs mainly in its oxidized form, Fe(III), in cores collected from upland locations in both the Lake Erie and Chesapeake Bay regions. In soil cores collected closer to the shoreline (i.e., forest transition zones and coastal wetlands), Fe is partitioned between Fe(III) and its reduced form, Fe(II), with Fe(II) proportions increasing from the intermittently flooded to the permanently flooded locations. Extended X-Ray absorption fine structure spectroscopy suggests that Fe(III) occurs as Fe-(hydr)oxide and Fe-bearing phyllosilicate minerals in both the Lake Erie and Chesapeake Bay regions. Thus, it appears that factors affecting Fe chemistry are similar in the two regions. In contrast, researchers observed the presence of Fe sulfides together with Fe-bearing phyllosilicate minerals in the Chesapeake Bay wetland soils, indicating a sulfur-driven redox chemistry, whereas Fe(II) is mainly observed in Fe-bearing phyllosilicate minerals at the Lake Erie sites. Complemented with mineralogical and porewater chemistry information, these results contribute to a better understanding of Fe redox cycling in saltwater and freshwater coastal systems.

Biogeochemistry and Function in Soils Transitioning from Coastal Forest to Wetland in the Chesapeake Bay

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Sea level rise drives spatial migration of coastal ecosystems and can lead to the replacement of coastal forests with tidal wetlands. Stressed or dead trees are well-recognized indicators of this conversion, but carbon (C) cycling, and soil biogeochemistry will also shift during this transition. Changes in soil biogeochemistry and vegetation during marsh migration may occur on different timescales, and this potential asynchrony will influence ecosystem function. Here, as a part of the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales—Field, Measurements,

and Experiments (COMPASS-FME) project, researchers determine how biogeochemical cycling of C and nutrients shift as upland coastal forests transition to tidal wetlands. Transects were established at four sites located throughout the Chesapeake Bay that represent spatial variation in elevation, soil types, vegetation, and salinity regimes. At each site, monthly measurements of soil methane (CH₄) fluxes, redox profiles, conductivity, and porewater constituents were made in upland forest, forest transitioning to wetland, and herbaceous tidal wetland transect locations. Despite live trees in the transition zone, researchers observed that soil biogeochemistry and function deviate strongly from conditions observed in the upland forest: along the gradient from upland forest to wetland, soils switched from a net sink to a net source of CH₄, soil redox potential decreased, and soil conductivity and porewater sulfate concentrations increased. The results indicate that transition zone soils begin to function similarly to tidal wetland soil prior to mass tree mortality, suggesting that by the time ghost forests are identified, soil function and biogeochemistry has already changed drastically. This has important implications for understanding the impacts of sea level rise and marsh migration on ecosystem-scale greenhouse gas emissions and C cycling across the terrestrial-aquatic interface.

A Multiscale Approach for Representing Integrated Hydro-Biogeochemical Processes Across Terrestrial Aquatic Interfaces

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The aquatic interfaces exposing terrestrial soils to oxic-anoxic regime shifts are hotspots of biogeochemical processes that are extremely sensitive to hydrological cycles and other external drivers. Interactions among water movement, physical heterogeneity, plant and microbial function regulate the transformations and fluxes of carbon (C), nutrients, and redox sensitive compounds. However, researchers lack a consistent, mechanistic modeling framework of these interactions or their scale dependency of hydrological, vegetation, and soil biogeochemistry that regulate whole-ecosystem function across terrestrial-aquatic interfaces

(TAIs). Researchers present a new modeling framework that connects a molecularly resolved biogeochemical model (AquaMEND) with surface and subsurface reactive transport modeling capabilities (via ATS-PFLOTTRAN) and the E3SM Land Model (ELM) to enable coupled process modeling across the soil-water-vegetation continuum. AquaMEND is a versatile biogeochemical model for solving dynamic coupling of organics, minerals and microbes from molecular to reaction and site scales. Leveraging bioenergetics as the central tenet governing microbial metabolic activities and C and nutrient fluxes, AquaMEND employs a flexible stoichiometry approach that accounts for microbial physiological traits, diversity of C substrate and dynamics of electron acceptors. High resolution FTICR-MS-based metabolomic data and metagenomes are used to generate energy balance for various reactions, which are further controlled by aqueous phase chemistry dynamically simulated in AquaMEND. Together, AquaMEND generates thermodynamically constrained reaction networks to provide ATS-PFLOTTRAN and ELM with lumped descriptions of the rates and efficiency of C and nutrient transformations. The resulting reaction networks and kinetics are then tested in PFLOTTRAN and incorporated into ATS-PFLOTTRAN for coupled hydrologic and biogeochemical modeling across upland-to-wetland transects.

Hydrological dynamics introduced by precipitation and tidal dynamics regulate solute distribution and oxygen dynamics, which exert additional controls on biogeochemical reactions. The coupling between hydro-biogeochemistry and vegetation dynamics is further realized through a three-column module of ELM, in which the impact of water level and salinity at the coastal TAI are explicitly represented for a C3 sedge (*Schoenoplectus americanus*, low marsh) and a C4 grass (*Spartina patens*, high marsh) plant functional types. Through the coupling of AquaMEND, ATS-PFLOTTRAN and ELM, local reactions, site-scale properties, and their interactions are fully integrated to enhance advanced modeling of coupled hydro-biogeochemical processes for holistic, predictive understanding of coastal TAI systems.

Other National Laboratory-Led Project

Early Career

Biogeochemical Processes Regulating Nutrient Solubility in a Freshwater Coastal Delta

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Coastal wetlands are undergoing rapid change in response to coastal degradation and sea level rise. On the Louisiana Gulf Coast, river management aimed at mitigating flood risk in urban areas has contributed to extensive land subsidence and the submergence of coastal zones. To maintain and restore these coasts, numerous projects are underway to divert river water and associated sediment loads into areas undergoing subsidence and salinization. The objective of this research is to evaluate how phosphorus (P) dynamics in coastal ecosystems are influenced by water management strategies that ultimately shape hydro-biogeochemical gradients. The initial phase of this project focuses on Wax Lake Delta (WLD), a nutrient-rich, freshwater delta that has formed recently as a result of water diversion away from the Mississippi River and into the Atchafalaya River. WLD is one of the few actively growing areas of coastal Louisiana

and is an example of ecosystems that could develop because of ongoing and future restoration projects.

The team's objective is to evaluate how P solubility shifts over time along redox gradients that develop in response to seasonal and tidal fluctuations in water level on the delta. Researchers have established two transects spanning supratidal to subtidal elevations on opposite ends of an emerging deltaic island that are comprised of either established (old) or newly formed (young) soils. Environmental sensors are being deployed to monitor redox potential, pH, and salinity at a high temporal resolution along each transect. Additionally, researchers are measuring a suite of biogeochemical parameters in surface and porewater.

Initial results from late autumn 2022 show that soils along the old transect were reducing at all depth levels and exhibited strong vertical gradients of nutrient solubility. Soluble reactive phosphorus (SRP) and ammonium were relatively low in surface water, $<0.06 \text{ mg L}^{-1}$ and $<0.4 \text{ } \mu\text{g L}^{-1}$, respectively, and increased up to 0.53 mg L^{-1} and 6.3 mg L^{-1} , respectively, by 30 cm in depth beneath the soil surface. In contrast, nitrate and sulfate concentrations were highest in surface waters yet strongly attenuated within the top 10 to 20 cm of soils. Researchers infer that reducing conditions within the soils result in nitrate and sulfate removal through anaerobic microbial metabolism, producing high concentrations of ammonium and sulfide. Moreover, increased phosphate solubility may be driven by reductive dissolution of metal oxides that otherwise bind P under oxidizing conditions. Ongoing evaluation of biogeochemical processes in WLD will improve process-based understanding of nutrient transformation in coastal ecosystems.

URBAN

Urban Integrated Field Laboratories

Southwest Urban Corridor Integrated Field Laboratory

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<https://sw-ifl.asu.edu/>

Arizona contains one of the fastest growing urban corridors in the U.S., including major cities of Tucson, Phoenix, and Flagstaff. With many of the region's urban areas routinely experiencing 30+ days of temperatures above 110 °F (43 °C) each summer, the population is stressed by the complex interactions of extreme heat, atmospheric pollutants, and limited water.

The Southwest Urban Corridor Integrated Field Laboratory (SW-IFL) will engage stakeholders and provide scientists and decision makers with high-quality, relevant knowledge capable of spurring and guiding responses to environmental concerns. The SW-IFL is a partnership involving the three public universities in Arizona, two national laboratories, and industry. The stakeholder network includes city governments, county-level agencies, community groups, and local nonprofits throughout the region.

The SW-IFL will specifically advance urban systems science by: (1) improving the understanding of how the built environment affects local to regional climates, emissions, and air chemistry; (2) establishing empirically grounded theory of how governance, actors, plans, and policies shape resilience to heat; (3) building a framework and simulation capability to facilitate equitable mitigation of extreme heat and its societal impacts; and (4) engaging government and community stakeholders in an advising and co-discovery role to drive the research process toward decision-relevant knowledge.

SW-IFL activities will include observations that leverage existing networks of weather, air quality, and hydrological measurements with new measurements of land-atmosphere exchange processes, atmospheric composition, and emissions. Intensive observational periods (IOPs) throughout the summer months will use mobile observatories to

measure boundary-layer processes, and focused neighborhood-scale heavily instrumented testbed experiments to elucidate drivers of microclimate variations and to evaluate the efficacy of proposed solutions. Testbed experiments will leverage data from the IOPs and include additional short- and long-term measurements that will engage researchers from across the university network and citizen scientists from the stakeholder organizations and communities.

Next-generation predictive modeling capabilities for urban regions will be developed by improving representations of fine-scale physical processes, while coupling existing state-of-the-art models that integrate human behavior and atmospheric phenomena ranging from neighborhood to regional and global scales.

The expected outcomes include integration of high-resolution observations (atmospheric, land surface, and infrastructure), diagnostic and predictive models, and civic engagement to provide new knowledge and deliver next-generation predictive tools that are regionally specific but also translatable to other arid regions. Ultimately, these tools will empower the public to respond to extreme heat, while informing development and deployment of policies and solutions that are effective, equitable and generalizable.

Southeast Texas Urban Integrated Field Laboratory: Equitable Solutions for Communities Caught Between Floods and Air Pollution

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<https://www.cae.utexas.edu/setx-uifl>

The Gulf Coast contains an extensive and diverse range of natural features and human settlements, with a disproportionate number of vulnerable communities. The region faces regular acute-on-chronic hazards in which short-notice technological and natural stressors (e.g., coastal storms, oil spills) occur alongside long-term/chronic environmental, industrial, and social stressors (e.g., subsidence, population growth, toxic pollution). This region will serve as a bellwether of change, providing either successful or failed adaptation of these compounded and coupled crises. However, addressing these challenges requires scientific understanding

in how the Earth system and the water cycle will change in the coming decades: (1) how anthropogenic alterations will affect the water cycle and air pollution through urbanization and human migration, water infrastructure, and land cover change; and (2) how community level green infrastructure intended to mitigate these stressors can in turn alter physical processes and the water cycle.

Researchers focus on the Beaumont-Port Arthur region, referred to herein as SETx-UIFL. This urban area represents the climate adaptation needs, population diversity and vulnerability, and ecological richness that characterize many urban centers along the Gulf Coast. Beaumont has experienced continued urban expansion and increased impervious cover over the past several decades; these changes have likely led to increased urban heat island effect and reduced capacity to absorb rainwater, exacerbating existing climate risk. In addition, the Beaumont, Port Arthur area is home to one of the nation's largest petrochemical industrial complexes, which make it more vulnerable to climate-induced disasters capable of significant air toxics releases in addition to chronic air toxic exposures that can raise the risk of cancer and other adverse health outcomes.

The main goal is to address the following questions: which processes and variables need to be captured in regional scale hydrological and atmospheric models so that they are representative of the conditions experienced by local communities and help inform adaptation strategies? And how can researchers understand the linkages between and within natural, built, and social systems in urbanized regions to better support natural and human resilience? These questions are addressed via three cross-cutting Themes (Environment, Co-design, Equity), which are linked through data collection strategies and community engagement supported by a Knowledge Management Platform (KMP). Three Activity Areas (AAs) coordinate activities across the Themes and KMP to ensure impacts are useful beyond the SETx-UIFL.

Community Research on Climate and Urban Science Urban Integrated Field Laboratory

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<https://www.anl.gov/crocus>

The Community Research on Climate and Urban Science (CROCUS) Urban Integrated Field Laboratory aims to advance urban science in the diverse, highly heterogeneous, human-altered Chicago region. It leverages existing, long-standing, and extensive observational and modeling capabilities from the team and empowers and actively involves diverse communities as part of the research team to facilitate just, long-term societal benefits from climate mitigation and adaptation. The Chicago region is nestled between the understudied but critically important Lake Michigan and former prairieland now converted to agriculture. Its socioeconomic and environmental inequalities are rooted in practices that date back to the early 1900s. CROCUS addresses science questions that have been formulated with critical community input. For example, how do urban environments influence urban heat islands; precipitation intensity, frequency, and duration; and uncertainties from the contrasting impacts of lake effects? How do neighborhood characteristics, vegetation, and soil properties influence the local climate? How can participatory, community-driven research integrate local knowledge with scientific processes to generate improved understanding of challenges, complexities, and aspirations of urban residents? To answer these questions CROCUS has developed a modular, portable, and scalable integrated ModEx architecture, inclusive of a micronet, specialized field campaigns, extensive collection

of existing data, and citizen science to support and interact with multiscale modeling. Information provided by communities frames a systems-based approach to evaluate different mitigation and adaptation technologies and scenarios and enables the understanding of the impact of these decisions on climate and communities. CROCUS investigates scalability from street-scale, local to global climate models, and researches best practices to address urban sustainability with distributed and equitable solutions.

Virtual

The Baltimore Social-Environmental Collaborative Integrated Field Laboratory

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The Baltimore Social-Environmental Collaborative (BSEC) seeks a new paradigm for urban climate research. Inspired by the Urban Integrated Field Laboratory (IFL) call to provide knowledge that informs equitable solutions that can strengthen community-scale resilience, BSEC proposes a people-centered, transdisciplinary IFL. BSEC begins with

community priorities (human health and safety, affordable energy, transportation equity, and others) and city government priorities (clean waterways, decarbonization, functioning infrastructure) and designs observation networks and models that will deliver the climate science capable of supporting those priorities. This means that BSEC takes the form of an iterative collaborative cycle, in which an initial observation and modeling strategy is continuously updated in conversation with community partners. The guiding objective of this cycle is to produce the urban climate science needed to inform community-guided “potential equitable pathways” for climate action. In doing so, researchers address a number of fundamental urban science questions from across natural and social science disciplines.

The BSEC Equitable Pathways approach aligns urban science with information needs through coupled cycles of model and observation improvement and participatory assessment of climate risks in the context of multiple, potentially competing priorities. Recognizing that city residents and institutions have diverse and sometimes competing goals, researchers place a multiobjective analysis tool at the center of their work. This analysis tool offers an integrating nexus to inform and challenge urban climate science with the decision needs of the residents and stakeholders who ultimately determine the success of climate action.

Additional Projects

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

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The heat island effect in urban environments is primarily associated with impervious surfaces and buildings that retain heat. However, the heat island effect can be moderated by natural ecosystem components such as soil moisture and tree evapotranspiration. Impervious surfaces and green space tend to be unequally distributed based on neighborhood economic value and social constructs such as redlining. The goal of this project is to understand how microclimates (e.g., temperature and relative humidity) in urban environments are affected by the activities of plant evapotranspiration and soil moisture. Soil moisture, the extent of impervious surfaces, and tree canopy are hypothesized to influence local microclimate. Specifically, low soil moisture, high percentages of impervious surfaces, and low extent of tree canopy will cause more intense heating in the summer and more intense cooling in the winter. Public parks in Knoxville, TN, were examined and three paired sites were chosen, with each pair having contrasting temperature, percent impervious surfaces, greenness, and social vulnerability. The paired sites have overall similar underlying geology, elevation, and soil water capacity to minimize confounding factors. The sites were instrumented with small weather stations, photosynthetically active radiation sensors, incoming and outgoing radiation sensors, and soil tension and soil moisture sensors, while trees were instrumented with sapflow sensors to serve as an indicator of evapotranspiration. Soil samples were collected for basic soil properties. The data will be used to determine relationships between urban microclimate and natural components (e.g., soil moisture and tree evapotranspiration) as a function of diurnal differences throughout the growing season. This research will be used to assess the utility of models in simulating the urban heat island effect with explicit consideration of natural ecosystem components.

Studying Urban Heat Island Effect Over New York City Using Satellite Observations, Ground-based Measurements, and Community Engagement

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The urban heat island (UHI) is among the major environmental issues encountered in urban regions. To better predict the dynamics of the UHI and its impacts on extreme heat events, an accurate characterization of the surface energy balance in urban regions is needed. However, the ability to improve understanding of the surface energy balance is limited by the heterogeneity of surfaces in urban areas.

This study aims to enhance the understanding of the urban surface energy budget and land surface temperature (LST) through an innovation in the use of remote sensing satellite observations and ground-based measurements. The research team conducts urban climate data collections using a suite of instruments such as flux towers, unmanned aerial vehicles (UAVs), infrared cameras, and hand-held temperature measuring devices. The team developed an algorithm to downscale a LST database with 5-minute temporal and 30-meter spatial resolution over New York City. Researchers also developed a model to identify cool corridors and open street paths as a resilient solution and response to UHI. A partnership with Brookhaven National Laboratory has been established through the DOE Research Development and Partnership Pilot funded project. The team is organizing a community field data collection for spring and summer 2023 in Manhattan and Brooklyn, NY. Finally, researchers will engage with the local community in Bedford-Stuyvesant neighborhood in Brooklyn, NY, in order to inform them about the urban heat island and to gauge its health and societal impacts.

CROSSCUTTING

At-Scale Molecular and Microstructural Analysis of Soil, Air, and Water Using the EMSL Molecular Observation Network

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<https://www.emsl.pnnl.gov/monet>

The Molecular Observation Network (MONet) is delivering a suite of new molecular and microstructural capabilities to the BER research community for understanding biogeochemical processes occurring within soils, air, and water across terrestrial-aquatic and terrestrial-atmospheric interfaces and at ecosystem and regional scales. The first major new capability was delivered in February 2023 with the launch of the MONet Soil Function soil core solicitation (<https://www.emsl.pnnl.gov/proposals/monet---soil-function-call/15039>). Soil cores submitted to the program will be analyzed for high-resolution composition of soil organic matter using Fourier-transform ion cyclotron resonance mass spectroscopy, 3D soil pore network structure using X-ray computed tomography combined with hydraulic property measurements, Illumina NovaSeq metagenome sequencing at the DOE Joint Genome Institute, and 20 additional critical soil biogeochemical parameters following standard workflows. Data will be available without embargo to the broad public in a findable, accessible, interoperable, reusable (FAIR) database that is searchable and provides visualization, mining, and manipulation tools.

The MONet program is a decadal strategic science objective at EMSL that reflects a commitment to delivering open network molecular ecosystems science opportunities at scale to the BER science community. Beyond the Soil Function call, MONet is developing automated soil molecular and microstructural analysis workflows for high-throughput analysis of soils at scale, rhizosphere sensors for quantifying small organic molecules in the laboratory and in field settings, and new methods for sampling atmospheric aerosols and particles at scale. Ultimately, MONet will enable new generations of experimental activities and multiscale models of Earth systems across entire regions.

Overview of Rhizosphere Function and Terrestrial-Atmospheric Processes Research at the Environmental Molecular Sciences Laboratory

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<https://www.emsl.pnnl.gov/science/expertise/rhizosphere-function/6>

<https://www.emsl.pnnl.gov/science/expertise/terrestrial-atmospheric-processes/3>

<https://www.emsl.pnnl.gov>

In 2023, EMSL launched two new Integrated Research Platforms (IRPs) to focus resources for molecular and microscale user research in critical ESS research domains:

Rhizosphere Function (RF) IRP: This program addresses the impacts of root system architecture and root exudates on highly interlinked rhizosphere components (e.g., microbial communities, organic matter, and soil mineralogy) in response to environmental perturbations. Supported research aims to dissect interactions between roots, the soil, and microbes to understand the impacts and mechanisms of root-controlled processes on plant resilience and biogeochemical cycling of carbon, nutrients, and mineral elements. Key capabilities include phytotrons, carbon flux using stable isotope probes and isotope-ratio mass spectrometry, synthetic soil habitats, quantitative cell imaging, molecular and chemical processes, and nondestructive measurement and imaging of root system architecture.

Terrestrial-Atmosphere Processes (TAP) IRP: This program addresses emission mechanisms of aerosols and gases from plants and soils into the atmosphere. It also addresses molecular processes that control the multiphase interfacial chemistry and aging processes occurring near Earth's surface and extending up to the atmospheric boundary layer. User research 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.

EMSL is a DOE Office of Science user facility sponsored by DOE-BER. The EMSL user science program supports fundamental biological and environmental research across the BER research domain, from bedrock to living organisms to the troposphere. Activities in the RF and TAP IRPs, and across the EMSL user program, are generating critical

observational data and model-based data to support Earth systems and climate models.

ESS-DIVE Overview: A Scalable, User-Focused Repository for Earth and Environmental Science Data

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<https://ess-dive.lbl.gov/>

The ESS-DIVE data repository stores diverse data from DOE-sponsored Earth and environmental research activities. The focus is on providing a scalable, robust repository for long-term curation of ESS data that adhere to findable, accessible, interoperable, and reusable (FAIR) principles. The repository currently focuses on three key areas: data access capabilities, services to support projects providing data to the repository, and data standardization. The approach is designed around user experience methods and involves significant discussion and involvement of the community in the design and development of capabilities. Repository priorities are continually revised and refined based on community input. Data access capabilities are continually being improved, including API-driven access and a new secondary storage layer to support very large hierarchical datasets. To meet the needs of a diverse set of projects, ESS-DIVE supports customized project-centric views of the data that enable grouped datasets to be displayed together, collaborative dataset management, and the ability to share datasets within a project. The use of data standards and reporting formats play key roles in enabling the broadest possible use of data. Nine community reporting formats have been developed to enable more structured files with descriptive metadata for diverse data types. This overview covers key features of ESS-DIVE and efforts to build a scalable, community-focused data repository.

Community-Developed (Meta)Data Reporting Formats to Enable Data Reuse in ESS-DIVE

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<https://ess-dive.lbl.gov/>

Earth science data are diverse and multidisciplinary, making it difficult for researchers to determine and use the appropriate standards or formats that apply to their data. The findable, accessible, interoperable, and reusable (FAIR) principles are intended to enable reuse of Earth and environmental science data beyond the purpose for which the data were originally collected. One pathway to making data more reusable is for repositories to encourage contributors to organize and publish data that follow established standards and guidelines. Twelve reporting formats are presented including instructions, templates, and tools for consistently formatting data for a diverse set of Earth science (meta) data. These formats were developed through a partnership between the ESS-DIVE repository and researchers from the ESS science community. They cover a broad range of Earth science (meta) data that includes cross-domain metadata (e.g., dataset metadata, location metadata, and sample metadata); file-formatting guidelines (e.g., file-level metadata, CSV files, and terrestrial model data); and domain-specific formats for biological, geochemical, and hydrological data types (e.g., amplicon abundance tables, leaf-level gas exchange, soil respiration, water and sediment chemistry, sensor-based hydrologic measurements, and unoccupied aerial systems). A community consensus process was

adopted to develop these formats by obtaining extensive input, resulting in a pragmatic set of reporting formats based on scientific use cases. Such community-developed reporting formats lend themselves to easy adoption, enabling scientific data synthesis and knowledge discovery by making it easier for data contributors to provide (meta)data that are more FAIR.

Focuses of the National Microbiome Data Collaborative

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<https://microbiomedata.org/>

The National Microbiome Data Collaborative (NMDC) is committed to providing findable, accessible, interoperable, and reusable (FAIR) multiomics microbiome data. This is accomplished through the three key NMDC products that are openly available to the research community: the submission portal (<https://data.microbiomedata.org/submission/home>), the data portal (<https://data.microbiomedata.org/>; Eloë-Fadrosh et al. 2022), and NMDC EDGE (<https://nmdc-edge.org/home>). The NMDC Submission Portal provides users a place to contribute sample metadata in a standardized manner with in-sheet validation to ensure machine readability and findability. The Data Portal consumes this metadata and presents search tools to find and access information about the research studies and data generated from the samples. The Data Portal also provides links to the associated omics data processed through NMDC's standardized bioinformatics workflows. NMDC EDGE is a user-friendly interface for NMDC standardized bioinformatics workflows. These three NMDC products are built specifically with the BER research community in mind and refined through a process of continual collaboration based on user-focused feedback. Leveraging each of the NMDC products enables environmental microbiome researchers

to adhere to FAIR data principles, thus expanding potential research questions, comparisons, and scientific discovery.

Eloë-Fadrosh, E.A., et al. 2022. "The National Microbiome Data Collaborative Data Portal: An Integrated Multiomics Microbiome Data Resource," *Nucleic Acids Research* **50**(D1), D828–D836. DOI:10.1093/nar/gkab990.

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From Snowflake to Snowpack: How Do Cloud Microphysical Process Representations Influence Hydrologic Response?

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The volume of water stored within seasonal snowpacks in the Upper Colorado River Basin is a fundamental constraint on downstream water availability. Climate change is already altering the partitioning of precipitation between rain and snow. Precipitation delivered as rain instead of snow bypasses a natural reservoir that delays its release and transits through fundamentally different pathways, having profound consequences for runoff production and biogeochemical cycling. Coupled land-atmosphere models are important tools that scientists use to examine effects of climate and climate change on precipitation. An important facet of modeling rain-snow partitioning in atmospheric models is how cloud microphysics are parameterized in these models, which simulate mass and the energy balance of hydrometeors based on important assumptions on their shape, size distribution, growth characteristics, and other properties. Here the project reports on numerical experiments examining the degree to which a variety of cloud microphysical process representations in the Weather Research and Forecasting (WRF) model leads to variability in spatiotemporal predictions of precipitation in the Upper Colorado River Basin. Within the East River Watershed, corresponding predictions of snow water equivalent and depth were created using the WRF-derived forcing scenarios as input to a land model and compared simulated snow conditions with retrievals from the Airborne Snow Observatory (ASO). Generally, more sophisticated

microphysics parameterizations produce better predictions of precipitation and snow water storage when compared to available precipitation and ASO data. Differences in simulated precipitation can, in part, be attributed to how vertical hydrometeor structure in the atmosphere is resolved. This study highlights the importance of atmospheric microphysics research for surface and subsurface hydrology and the role that snowpack, and in general, surface observations can play in constraining atmospheric processes and advancing atmospheric science research. Field campaigns—like DOE’s Watershed Function science focus area—that collect intensive and temporally extensive hydrologic and critical zone data are collocated with campaigns like the Surface-Atmosphere Integrated Laboratory, which collects intensive near-surface atmosphere data, hold promise for co-producing scientific insights that are mutually beneficial to both fields.

The National Virtual Climate Laboratory Portal

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NVCL.energy.gov

BER is supporting the National Virtual Climate Laboratory (NVCL) portal to allow those who have a stake in the climate crisis to access the capabilities, research, and facilities that reside in DOE national laboratories and user facilities. The portal is designed to be transparent, agile, content-rich, and user friendly and to enable more efficient engagement with DOE’s science and technology. The portal will also enhance the national laboratory system’s relationships with and visibility to educational organizations, in particular minority-serving institutions (MSIs) by offering insights into research activities that could provide collaborative opportunities and pathways to training and career development to build a next-generation climate workforce. The NVCL portal has three major objectives: (1) centralize climate research information conducted at the national laboratories on BER’s Earth and Environmental Systems Sciences Division (2) institute a well-curated, easily accessible, plain-language inventory of DOE facilities, projects, and BER news related to climate research that will be available for students, scientists, faculty and other interested entities; and (3) facilitate strong collaborations between the national laboratories and interested organizations, especially MSIs. The overarching goal is to broaden the understanding of research activities and facilitate the design and development of internship and training programs. The portal will be updated continuously as a living document.

Early Career

Urban Resilience Across the Terrestrial-Aquatic Continuum

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Over 70% of the world’s population is predicted to live in urban areas by the end of the century, yet the impacts of urbanization on ecosystem functions remain ambiguous. This contributes to high uncertainty in the representation of urban carbon (C) cycling within Earth Systems Models, which in turn leads to imprecise predictions of the global climate. In particular, ecosystems across the urban terrestrial-aquatic continuum have an outsized impact on global C cycles but are poorly understood. Across the terrestrial-aquatic continuum, urban land uses contribute excess C and nutrients (nitrogen and phosphorous) to soils and waterways, which in turn regulate microbial C cycling. Precipitation heightens these impacts by flushing materials into aquatic ecosystems and, ultimately, into the coastal ocean.

The goal of this research is to identify locations exerting strong impact on C biogeochemistry (i.e., control points) and then understand the interplay of molecular controls, nutrient supply, and hydrologic factors that fuel rapid microbial C processing at these locations. The team’s hypothesis is that commonalities in microbial functions lead to conserved control points and biogeochemical processes that are distinct to the urban environment and regulate organic matter (OM) decomposition across its terrestrial-aquatic continua. To achieve these outcomes, the team will employ top-down (non-target) and bottom-up (targeted towards specific genes) molecular analyses to identify enzymatic pathways of OM decomposition impacted by anthropogenic activities, structured to integrate into microbial-explicit models. This molecular understanding is critical for improving the predictive abilities in novel environmental scenarios as it drives the relative magnitudes of the various C cycle fluxes at the ecosystem-to-Earth system scale. Collectively, this work will create a unique knowledge set inclusive of control points, microbial OM decomposition processes, and their relationships to various urban attributes that influence the response of coastal zones to environmental extremes.

Genomic Resources for Advancing Environmental System Science

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jgi.doe.gov

The DOE Joint Genome Institute (JGI) is a large-scale genomic science user facility dedicated to advancing discovery and innovation in support of DOE's mission areas in energy and the environment. The JGI provides users around the world with access, at no cost, to high-throughput genomic capabilities for microbes, microbial communities, plants, and fungi. In Fiscal Year 2022, the JGI served a worldwide community of 2,243 users from academia, government, and industry. These proposals include genome, transcriptome, metagenome, metatranscriptome, and single-cell sequencing; resequencing; DNA synthesis; and metabolomics. In support of these proposals, JGI produced sequencing output of 658 trillion nucleic acid bases. These data enabled high-impact science from the user community, yielding 252 publications through support and complementary efforts by the JGI Science Programs.

DOE X-Ray Light Sources, Neutron Scattering, and Cryo-Electron Microscopy User Capabilities for Environmental System Science

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<https://BERStructuralBioPortal.org>

<https://science.osti.gov/bes/suf/User-Facilities>

The BER ESS program seeks to advance an integrated, robust, and scale-aware predictive understanding of terrestrial systems and their interdependent microbial, biogeochemical, ecological, hydrological, and physical processes. Structural and chemical insights at the atomic, molecular, and mesoscale levels are critical for developing multi-scale, multi-component models that can be used to predict system behavior and inform process knowledge and systems models. These insights advance the goals of the ESS program to understand the ecological and hydro-biogeochemical linkages among system components and to characterize the complex processes and controls on the structure, function, feedbacks, and dynamics of terrestrial ecosystems and watersheds.

A wide array of synchrotron-, neutron-, and electron-based techniques are available for characterizing structure, function, and interrelationships among complex molecular components that are relevant to ESS. The spatial and temporal resolutions available from neutron, photon, and electron beams enable characterization and imaging of system components and interactions among plants, microbes, water, and soil constituents (organic and mineral). Accessible scales range from subnanometer to centimeter length and time dimensions from femtoseconds to seconds and longer.

Capabilities and resources at the DOE synchrotron and neutron facilities, especially suited for ESS, provide expert guidance, user support, and training for designing experiments and measuring data. Cryo-electron microscopy and tomography are also available techniques. Free access is available for competitive proposals. Please visit the poster and peruse the informational brochures.

The X-ray light sources and neutron scattering facilities are constructed and operated by the DOE Office of Science, Basic Energy Sciences Scientific User Facility Division. The BER Structural Biology and Imaging User Resources at the DOE Basic Energy Science facilities and at EMSL are operated by BER.

Leveraging the AMF3 Campaign to Target Land- Atmosphere Interactions and Study Regional Heterogeneity in the Southeast United States

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The upcoming redeployment of the U.S. Department of Energy Atmospheric Radiation Measurement (ARM) third mobile facility (AMF3) to the Southeastern United States, with siting focused on Northern Alabama, will provide unprecedented opportunities study aerosol, cloud, and land-atmosphere interactions (LAI) in a region with strong local surface-atmosphere coupling and feedbacks. A major focus of the campaign will be detailed studies into the roles surface processes (e.g., momentum, heat, CO₂, biogenic volatile organic compounds, and water vapor fluxes) and land-surface heterogeneity play on boundary layer dynamics and larger, regional-scale weather patterns, as well as critical two-way interactions between atmospheric conditions and vegetation function. To facilitate this research, the AMF3 Site Science Team (SST) has been engaged with ARM,

AMF3 operations partners, and the larger scientific community to guide the siting, configuration, and instrumentation required to address these core research areas. The expected surface and LAI observation network for the AMF3 deployment will include a heavily instrumented main-site tower facility, located in a representative forested region to observe important vertical and ecosystem-scale processes that influence local weather, as well as spatially distributed supplemental sites to facilitate regional-scale surface-atmosphere studies. This planned surface observation network will be linked with multiscale, multidomain (e.g., aerosol, cloud

processes) spatial datasets and modeling activities to explore methods for upscaling surface measurements to the larger region and study connections with atmospheric processes. The SST is also engaged in pre-deployment activities to develop a baseline understanding of the Southeast U.S. region and identify optimal sampling strategies for surface-aerosol studies. Importantly, the location of the AMF3 deployment will also offer important partner agency and university collaborations to enhance the LAI focus, including proximity to other surface measurement networks (e.g., NEON, AmeriFlux, IMPROVE)

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