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

U.S. DEPARTMENT OF ENERGY | Office of Science
Office of Biological and Environmental Research

Title: **The Last Glacial History of the East River Valley, Colorado: Implications for Watershed Function**

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

BER Program: ESS

Project: Early Career project

Project Abstract: The geomorphic history of watersheds can influence watershed function by altering topography, subsurface flow paths and hence the timescale of mineral-water interactions. Erosion can also remove the critical zone, thereby re-setting the template for chemical weathering. In mountain landscapes, like the East River watershed near Crested Butte, Colorado, the extent, timing, and intensity of past glaciations can have long lasting impacts on watershed processes. However, relatively few investigations of ancient glaciations have occurred in the East River watershed and none have used modern cosmogenic exposure dating techniques. Here we present, >20 new *in situ*-produced ^{10}Be exposure dates for glacial landforms in the East River and Washington Gulch valleys. The exposure dates provide limits on the timing and extent of the most recent glaciation, which is globally known as the Last Glacial Maximum (LGM) and locally termed the Pinedale glaciation, and the rates of deglaciation. We also use ice-flow modeling to constrain the parts of the watershed that were ice-covered and ice-free during the LGM. The distribution of moraines and ice modeling results indicate glaciers from the East River crossed the drainage divide and flowed into Washington Gulch. The summit of Snodgrass Mountain extended above the maximum elevation of glaciation, and hence may have a much thicker and well-developed weathering zone than adjacent areas that were incised by glacial erosion. The ^{10}Be ages, currently undergoing analysis at Lawrence Livermore National Lab, will constrain the timing of glaciation and ice retreat, and hence provide a spatially averaged view of the time at which bedrock in the watershed was first exposed to weathering. In addition to constraining the time weathering initiated in different parts of the watershed, establishing the timing of glacial moraine deposition is a key part of our overall project, as dating the moraines and sampling soils will allow us to calibrate the deposition rate of meteoric ^{10}Be within the watershed. Calibration of the delivery rate to soils is required to use meteoric ^{10}Be to infer erosion rates in non-quartz-bearing lithologies, and we intend to apply this technique to the portions of the watershed with Mancos Shale bedrock.

Title: Oscillating Redox Conditions Controlled Greenhouse Gas Dynamics in Wet Tropical Forest Soils

Melanie A. Mayes[1]*, Debjani Sihi[1], Jianqiu Zheng[2], Julia Brenner[1], Jana Phillips[1], Shikha Singh[3], Jennifer Pett-Ridge[4], Sindhu Jagadamma[3], and Carla López Lloreda[5]

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BER Program: ESS

Project: Early Career Award

Project Website: n/a

Project Abstract: Wet tropical forest soils can oscillate between fully oxygenated and fully anoxic conditions, which can differentially influence the dynamics of greenhouse gases such as carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O) as a function of landscape topography. To gain a better understanding of in situ processes, we mimicked the dynamic redox oscillations in a laboratory incubation using soil samples collected from valley and slope positions along a catena near the El Verde Field Station, Luquillo Experimental Forest, Puerto Rico. Sixty grams of fresh soil was incubated under static oxic, static anoxic, and alternating redox conditions (every 4 days) over 76 days. The dynamics of greenhouse gases, redox-sensitive elements (total/reduced iron, ammonium, nitrite, and nitrate), extractable organic acids, pH, microbial biomass, hydrolytic enzymes, dissolved organic carbon, and organic/inorganic phosphorus were monitored. Overall, net CO_2, CH_4, and N_2O fluxes followed the pattern of alternating > oxic > anoxic, anoxic > alternating > oxic, and oxic > alternating > anoxic treatments, respectively. We observed higher reduced iron concentrations under the anoxic treatment and in the valley soils. Soil pH partially followed the pattern of reduced iron, especially for the anoxic treatment. Valley soils had greater nitrate than slope soils, especially under the oxic treatment. Landscape topography exerted an opposite effect on microbial biomass phosphorus, where valley > slope, and phosphorus-degrading enzymes phosphatase and di-phosphatase, where slope > valley. However, microbial biomass phosphorus and phosphorus-degrading enzymes followed a similar pattern under redox treatments (oxic > alternating > anoxic). Hence, both redox conditions and landscape topography influenced soil biogeochemistry and altered greenhouse gases dynamics. We used a geochemical modeling

framework, PHREEQC, to represent the tight coupling and rapid dynamics of carbon, nitrogen, phosphorus, and iron cycles and associated greenhouse gases dynamics in wet tropical forest soils. This research will aid in understanding and predicting the high degree of variability of greenhouse gas emissions in tropical climates.

Title: **Tropical Forest Response to a Drier Future: Synthesis and Modeling of Soil Carbon Stocks and Age**

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Project Lead Principal Investigator (PI): Karis McFarlane

BER Program: TES

Project: Early Career project

Project Website: na

Project Abstract:

Tropical forests account for over 50% of the global terrestrial carbon sink and 29% of global soil carbon, but the stability of carbon in these ecosystems under a changing climate is unknown. Recent work suggests moisture may be more important than temperature in driving soil carbon storage and emissions in the tropics. However, data on belowground carbon cycling in the tropics is sparse, and the role of moisture on soil carbon dynamics is underrepresented in current land surface models limiting our ability to extrapolate from field experiments to the entire region. We measured or attained data for soil carbon stocks and radiocarbon (14C) values of profiles from over 40 sites spanning 12 pan-tropical regions. Our 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. We found a large range in soil 14C profiles between sites, and in some locations, we also found a large spatial variation within a site. MAP explains some of the variation in soil 14C profiles and carbon stocks, with smaller C stocks and younger soil carbon in drier forests. However, differences in soil type contribute substantially to observed variation across the dataset and with constrained gradients in moisture and parent materials in Panama. We are exploring the influence of controlling factors in manipulation experiments and constrained gradients of precipitation, soil type, root inputs, geomorphology, and landuse on carbon storage and longevity through collaborative site-specific studies. For example, conversion of primary forests to pasture in the Ucayali region of Peru caused a loss of young soil carbon in 10-20-year-old pastures. Reforestation of agricultural lands restored young soil C stocks after 15 years, but these forests retain a legacy of lost carbon. Site-level runs of ELM v.1 and integration with a reduced complexity model (SoilR) are being used to evaluate model representation of soil C processes, including vertically-resolved carbon transfer rates, root inputs, and decomposition. In comparing measured soil C stocks and 14C profiles to data generated from ELMv1, we found

that the model continues to overestimate carbon stock and underestimate turnover time. Finer resolution runs of ELMv1 and site-level model-data comparisons will provide more insight and be used to assess the role of climate vs other soil (e.g., soil type and parent materials) and ecosystem factors (e.g. rooting depth) in driving vertically-resolved measured and modeled soil carbon pools and ages.

LLNL-ABS-807370

Title: Understanding the microbial controls on biogeochemical cycles in permafrost ecosystems

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Project Lead Principal Investigator (PI): Neslihan Taş

BER Program: Genomic Science

Project: Early Career Research Project

Project Abstract:

This project use state of the art molecular techniques to resolve complex microbial processes governing the biogeochemical cycles in arctic soils and permafrost to better inform efforts to access uncertainties surrounding ecosystem responses. Permafrost soils are one of the world's largest terrestrial carbon storages thus an important focal point for climate change research. With increasing global temperatures, permafrost carbon stores may become available for rapid microbial mineralization and result in increased greenhouse gas (GHG) emissions. Upon permafrost thaw microbial metabolism leads to decomposition of soil organic matter, substantially impacting the cycling of nutrients and significantly affecting the arctic landscape. Permafrost microbiome is a seed bank of mostly novel organisms that have a diverse and broad metabolic potential. In-depth functional characterization of the permafrost microbes is needed to provide a foundation for understanding their responses to thaw. In order to address this gap in our knowledge we performed a pan-Arctic comparative analysis of permafrost metagenomes in which we study biogeography and metabolic functions of permafrost metagenomes assembled genomes (MAGs). This pan-Arctic analysis of permafrost MAGs across multiple locations showed weak correlations to environmental conditions (ice content, topography, continuity, active layer depth, and vegetation) or soil chemistry.

The microbial response to thaw in arctic environments is not uniform and the relationship between permafrost microbiomes and GHG emissions is not well understood. Especially the fate of carbon in deep permafrost, which is currently protected from the warming climate, is uncertain. Following thaw, redistribution of water is a key event that conditions the permafrost for microbial decomposition. We tested the impact of soil moisture availability under microaerophilic and anaerobic conditions via small scale batch experiment. We couple omics (metagenomics and metatranscriptomics) methods with analysis of soil chemistry via synchrotron fourier transform

infrared (sFTIR) spectral imaging at the Berkeley Infrared Structural Biology beamline of the Advanced Light Source (LBNL). Upon thaw variety of organic compounds and metabolites were accumulated. For example, under saturated high-moisture conditions carbohydrates were depleted and soils accumulated aliphatic compounds. This microbial response was tied to the competition between methanogenesis and iron and/or sulfate reduction processes. This project use field observations, laboratory manipulations, and multi-omics approaches to examine how microbial processes, biogeochemical transformations, and hydrology interact during permafrost thaw in different sites in Alaska in order to determine how these factors drive biogeochemical cycles.

Title: Towards a Mechanistic and Predictive Understanding of Reactive Nitrogen Oxide Fluxes to and from Soil

Authors: Jonathan D. Raff[1,2,3]* Ryan M. Mushinski[1,3,4], Adrien Gandolfo[1,3], Clara Lietzke[2], Richard P. Phillips[4], Zachary C. Payne[2], Cheng Zhu[2], Rebecca Abney[1,3], Sally E. Pusede[5], Douglas B. Rusch[6], Jeffrey R. White[1,3], Lane Baker[2]

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

BER Program: ESS

Project: University project, Early Career project

Project Abstract:

Nitrogen (N) cycle processes play a crucial role in regulating the overall abundance of oxidized inorganic nitrogen in terrestrial ecosystems, and are responsible for initiating the subsequent loss of soil N via volatilization and leaching. This poster will outline our laboratory's effort to understand the sources and sinks of reactive nitrogen oxides (NO, NO_2, HONO, and N_2O) with the goal of improving model parameterizations in chemical-transport models that include terrestrial-atmospheric interactions. The study uses a combination of field and laboratory measurements to study gas-surface exchange of these reactive gases on the landscape to the molecular level. At the landscape scale, we used soils collected from temperate forests across the eastern United States to show that microbial communities involved in nitrogen (N) cycling are structured, in large part, by the composition of overstory trees, leading to predictable N-cycling syndromes, with consequences for emissions of volatile nitrogen oxides to air. Trees associating with arbuscular mycorrhizal (AM) fungi promote soil microbial communities with higher N-cycle potential and activity, relative to microbial communities in soils dominated by trees associating with ectomycorrhizal (ECM) fungi. Metagenomic analysis and gene expression studies reveal a 5 and 3.5 times greater estimated N-cycle gene and transcript copy numbers, respectively, in AM relative to ECM soil. Furthermore, we observe a 60% linear decrease in volatile reactive nitrogen gas flux (NOy = NO, NO_2, HONO) as ECM tree abundance increases. Currently, we are following

up on this study with in situ measurements of N_2O and CO_2 in local hardwood forests in an effort to determine whether fluxes measured in laboratory microcosm experiments are comparable to those measured in the field. Finally, results of a new study of the mechanism of HONO release from soil clay mineral surfaces at the molecular level will be presented. Specifically, the surface acidity of kaolin minerals was probed using scanning conductance ion microscopy for the first time. Steps and edges consisting of incompletely coordinated aluminum hydroxide groups were found to be likely reactive sites that are responsible for the release of nitrite as HONO to the atmosphere at soil pH well above the pK_a of nitrous acid.

Title: Global Trait-Based Chemogeography of Organic Matter Thermodynamics

Aditi Sengupta,[1] Vanessa Garayburu-Caruso,[2] Sarah Fansler,[2] Rosalie Chu,[3] Robert Danczak,[2] Marci Garcia,[2] Amy Goldman,[2] Emily Graham,[2] Matt Kaufman,[2] Lupita Renteria,[2] Daniel Sandborn,[2] Hyun Song,[4] Josh Torgeson,[2] Jason Toyoda,[3] Coastal Consortium,[5] WHONDRS Consortium,[6] and James Stegen[2*]

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Project Lead Principal Investigator (PI): James Stegen

BER Program: Other

Project: Early Career

Project Abstract: *This study is part of an Early Career project focused on transforming our ability to understand and predict how the influences of biogeochemical hot spots and hot moments on surface–subsurface systems are altered by perturbation. New theory and models are being developed across a broad range of watersheds to ultimately inform next-generation Earth system models and help preserve long-term national clean water security.* River corridors are fundamental to global elemental cycles, and thermodynamic traits of organic matter (OM) underpin biogeochemical processes in these ecosystems. Theory allows use of OM thermodynamics in predictive models, but is limited by knowledge gaps associated with trait chemogeography and relationships among traits. We used globally crowdsourced samples to address this need. We reveal latitudinal and longitudinal trait gradients in both inland and coastal river corridors. Global relationships among traits indicate first-order constraints tied to a universal tradeoff based on thermodynamic controls over the efficiency of converting OM into biomass. River water and sediment OM diverge markedly in their position along this tradeoff axis. Large scale chemogeography and universal trait relationships enable inclusion of OM thermodynamics in predictive models across scales.

Linkages Between Hydrologic Processes and Biogeochemical Cycling in Salt Marshes

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BER Program: ESS
Project: University Award (DE-FOA-000218)
Project Website: http://mzimmer.weebly.com/nitrates.html

Salt marshes exist at the terrestrial-aquatic interface between watersheds and the ocean. These tidal systems are hot spots of biogeochemical activity within coastal watersheds. Yet, we have limited understanding regarding how short-term (e.g. daily tidal cycles) and long-term (e.g. seasonal precipitation and climate patterns) hydrologic forcings may interact within these systems. These interactions will affect the temporal dynamics, or hot moments, of nutrient processing as well as the physical zonation of biogeochemical processing in the subsurface, or hot spots. To address this knowledge gap, we instrumented a ~25 m transect along a representative salt marsh platform at the Elkhorn Slough National Estuarine Research Reserve in California, USA. We installed variable-depth redox probes, nested piezometers, and a field-deployable spectrophotometer with a multi-source pump at lower, mid, and upper marsh positions to allow for characterization of subsurface hydrologic cycling and dissolved inorganic nitrogen (DIN) species concentrations at a high frequency (~15 min). We also conducted seasonal sediment incubation experiments to quantify nitrogen processing rates. We found that DIN concentrations fluctuated hourly due to frequent tidal flushing that introduced oxygen and ammonium-rich surface water into sediments under reduced conditions, with the largest change in concentrations observed in lower marsh positions. Sediment core incubations showed a dominance of net N_2 flux out of the marsh, indicating removal by denitrification, but the impacts of seasonal and event-driven freshwater contributions affected elevations differently, with the largest changes seen in upper marsh positions. Together, our findings suggest that intra-annual changes in source water contributions across the marsh result in functional zonation, where lower marsh position functions may be regulated by tidal flushing and upper marsh position functions may be regulated by freshwater contributions.

A data-driven approach to predicting the impacts of hydrometeorological disturbances on water quality in river corridors

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BER Program: ESS

Project: Early Career Project

Project Website: http://sites.google.com/lbl.gov/inaiads

Project Abstract:

Hydrometeorological disturbances such as floods, droughts, and heatwaves are projected to increase over the next few decades due to climate change. These disturbances can worsen water quality by impacting water temperature and salt, nutrient, contaminant concentrations, which will have direct consequences for human and ecosystem health. Hence, it is important to understand and predict how water quality in streams and rivers will respond to new disturbance regimes. Here we describe results from a U.S. Department of Energy (DOE) early career project that utilizes data-driven approaches to understand how these climate-induced disturbance events impact water quality over time. Our study is focused on water temperature and conductivity (salinity) predictions in three U.S. hydrological regions - the mid-Atlantic, Pacific Northwest and Upper Colorado. First, we present the use of low-complexity machine learning models (Multiple Linear Regression, Support Vector Regression, and Random Forest Regression/XGBoost) to predict monthly stream water temperature at the point to watershed to regional scales. We compare the performance of these models between basins with differing climate, geological, land use and water management attributes. In particular, we focus on improving model performance by separating free-flowing and dammed stream reaches, and by grouping stations by their time-series dynamics. Next, we present results from analysis of change in regional water temperatures during heat waves. Finally, we present the iNAIADS framework (iNtegration, Artificial Intelligence, Analytical Data Services) which comprises a data integration tool BASIN-3D (https://basin3d.readthedocs.io/) that can be used to reproducibly synthesize diverse data from distributed sources, along with reusable analytical and machine learning codes.

Transport and Retention of Motile Microbes in Pore Networks: Progress and Plans

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BER Program: SBR

Project: EPSCoR

This project seeks to understand the motion and retention dynamics of motile microbes at the micro- and pore-scale and utilize upscaling techniques to study impacts of microbial motility on metal bioremediation simulations at the field-sale. A series of experiments with motile bacteria, using microfluidic devices and advance imaging techniques, were conducted (and are planned) to quantify the fundamental character of bacterial motion in porous media during active swimming. The experiments form the basis for development and testing of new models of microbial transport and retention. Trajectories of individual cells for several metal reducing species were analyzed to provide information on the length of runs, and time needed to complete a run. These motion statistics were used to construct a continuous time random walk model and its performance in reproducing real breakthrough plots were compared against traditional modeling approaches based on the advection diffusion equation. We have further employed random walk particle-tracking (RWPT) approaches to elucidate the impact of porous media confinement and cell-cell interactions on the overall bacterial transport. We validated our RWPT model against single-cell resolution data from 3D porous media which showed that the model can efficiently simulate the spreading dynamics of motile bacteria in confined geometries. More recently, we have extended our micromodel experiments to study spatial organization of biofilms in pore networks and evaluate the impact of biofilm-induced flow heterogeneities on conservative transport. Biofilm images were processed to represent them as a synthetic porous structure in numerical models. With biofilms present, we observed enhanced solute spreading in breakthrough curves that exhibit extreme anomalous slopes at intermediate times and very marked late arrival due to solute retention. We are currently integrating micro-scale models with pore-scale simulations and using it to generalize and upscale microbial transport to a broader range of pore geometries and flow conditions. In the coming months, the results of pore-scale simulations will be used to parameterize effective transport and retention properties for field-scale models of microbial transport that can be incorporated into existing simulators of metal bioremediation.

Building a Culture of Safety and Trust in Team Science

Colleen Iversen[1*], Katrina Bennett[2], Robert Bolton[5], Amy Breen[5], Baptiste Dafflon[3], Ranjeet Devarakonda[1], David Graham[1], Sue Heinz[1], Susan Hubbard[3], Alistair Rogers[4], Vladimir Romanovsky[5], Joel Rowland[2], Peter Thornton[1], Margaret Torn[3], William Riley[3], Cathy Wilson[2], and Stan Wullschleger[1]

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BER Program: ESS

Project: NGEE Arctic

Project Website: https://ngee-arctic.ornl.gov/

Project Abstract:

Some of the most scientifically exciting places are also some of the most difficult to study. The Arctic, for example, is rapidly changing, as evidenced by melting sea ice, thawing permafrost, disappearing glaciers, and greening hillslopes. Increasingly, scientists from around the world and across a wide spectrum of disciplines are working together to advance our understanding of this vulnerable and globally important biome. As scientists become part of larger teams and join broader and more diverse scientific endeavors, they must all become leaders in creating cultures of safety, inclusion, and trust to facilitate the physical and emotional well-being of individuals in scientific teams and in the local communities where scientists work. Here we share lessons learned from an "experiment within an experiment" begun as part of a large-scale, decade-long research project in Alaska. The experiment was focused on answering the question: How can we intentionally create a project-wide culture of safety, inclusion, and trust that facilitates strong cross-disciplinary collaboration and exciting scientific discoveries?

Our team of more than 150 people includes empiricists, modelers, and data scientists from four U.S. Department of Energy National Laboratories as well as from the University of Alaska Fairbanks (UAF), all working together on the Next-Generation Ecosystem Experiments–Arctic (NGEE Arctic) project. We achieve our scientific goals by underpinning our science with a strong culture of safety, inclusion, and sharing: (1) We make the safety of ourselves and our team our number one concern before, during, and after field and laboratory campaigns by encouraging

rigorous planning, continuous dialogue, and questioning attitudes. (2) We hold each other accountable by promoting a respectful and harassment-free work environment for everyone, both within the project team and within the broader community of local and indigenous people where we are guests. (3) We prioritize cross-disciplinary collaboration through project-wide sharing of ideas—from senior researchers to first-year students—facilitated by a system to openly and immediately share data, both within the project and beyond. (4) We continue to learn by engaging with each other in planning exercises that span the 'what ifs' of scenarios that could endanger team member physical or emotional safety, by engaging with other projects on their own codes of conduct at annual meetings, and by inviting speakers from programs like ADVANCEGeo to help us understand the pitfalls of implicit bias and to improve our project culture.

References:

Iversen, C. M., W. R. Bolton, A. Rogers, C. J. Wilson, and S. D. Wullschleger (2020), Building a culture of safety and trust in team science, Eos, 101, https://doi.org/10.1029/2020EO143064. Published on 21 April 2020.

The AmeriFlux Management Project: Overview

Margaret S. Torn,[1*] Deb Agarwal,[1] Dennis Baldocchi,[2] Sebastien Biraud,[1] Stephen Chan,[1] You-Wei Cheah,[1] Danielle S. Christianson,[1] Trevor Keenan,[1,2] Housen Chu,[1] Sigrid Dengel,[1] Marty Humphrey,[4] Fianna O'Brien,[1] Dario Papale,[3] Gilberto Pastorello,[1] Christin Buechner[1]

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Project Lead Principal Investigator (PI): Margaret S. Torn

BER Program: TES
Project: AmeriFlux Management Project (lead: LBNL)
Project Website: http://ameriflux.lbl.gov/

Project Abstract:
AmeriFlux is a network of sites and scientists measuring ecosystem carbon, water, and energy fluxes across the Americas using eddy covariance techniques. The DOE AmeriFlux Management Project (AMP, established 2012) works to enhance the value of AmeriFlux for Earth system modeling, terrestrial ecosystem ecology, remote sensing, and many other fields. As of June 2021, more than 540 sites have joined the AmeriFlux and quality-assured data can be downloaded for nearly 400 of these. These sites represent a wide range of climate and ecological conditions, natural disturbance, and land management. AMP supports operations of 13 core-sites teams (44 sites) to provide high-quality, long-term data; (2) provides technical support and site visits to enable inter-comparison and synthesis of data across sites; (3) quality assesses data and produces standardized data products for basic research, resource-management applications, and Earth system model (ESM) improvement; and (4) holds virtual community meetings and webinars.

Highlights from the past year include: creating a more open data policy, based on CC BY4, with participation of more than half the sites already; releasing a beta FLUXNET product for 63 sites; holding a virtual community meeting with attendees from 32 countries. AmeriFlux BASE (flux/met) data were downloaded by 1,310 users and the new webinar series had cumulative attendance of more than 1200 people and 1500 YouTube views. Finally, in March AmeriFlux launched a new theme year for network action –The Year of Water Fluxes—with broad community engagement and connections to interagency activities.

Title: AmeriFlux Community Initiatives - Water Year, FLUXNET, Urban Fluxes, and More!

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BER Program: TES

Project: AmeriFlux Management Project (lead: LBNL)
Project Website: http://ameriflux.lbl.gov/

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

As part of our community collaboration initiatives, we host theme years of focal interest. This year, we launched the Year of Water Fluxes as our next theme year for community action. There are many science opportunities to study water fluxes in AmeriFlux. This theme year will support more water cycle measurements, enhance data quality, and build strong collaborations to work on the various aspects of water and fluxes. Initial activities in the space include a land-atmosphere interactions workshop focused on atmospheric boundary layers and relationships with water and carbon fluxes (June 10/11th) (https://ameriflux.lbl.gov/community/ameriflux-meetings-workshops/) and a water focused AmeriFlux Annual Meeting. More activities and opportunities for engagement with the community are planned over the coming year.

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

There is a growing interest in using the eddy covariance technique in urban environments. Compared to natural and working lands, there is limited knowledge on using eddy covariance to generate robust estimates of urban land fluxes. We have assembled a working group of 10 experts in urban fluxes to distill applications, challenges, and recommendations for eddy covariance measurements in urban environments. They will also consider how eddy flux could contribute to the proposed Urban Integrated Field Laboratory. The committee, which held its kick-off meeting in April 2021, will produce a brief white paper to share with BER and the AmeriFlux community.

Title: New (and Improved!) AmeriFlux Data Products and Services for Earth Science Research

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BER Program: TES

Project: AmeriFlux Management Project (lead: LBNL)
Project Website: http://ameriflux.lbl.gov/

The AmeriFlux Management Project (AMP) disseminates standardized flux/met and ancillary data products from 394 AmeriFlux sites. Over 230 sites have elected to release their data under the CC-BY-4.0 data license, also adopted by most sites in FLUXNET2015, which was updated in February 2020. AmeriFlux data distribution under this new license will begin in 2021. An open data policy allows for more streamlined data sharing while still giving attribution to site teams via data DOI citations.

The *AmeriFlux BASE data product* is continuous half-hourly/hourly quality-controlled flux and meteorological (flux/met) data provided by site teams and formatted in the Flux Processing (FP) global standard. Data for each site is assigned a DOI. Data users can search over 2,600 site-years of BASE data by 133 variables spanning 30 years (1991-2021) on the AmeriFlux website. Supporting Biological, Ancillary, Disturbance, and Metadata (BADM) are also available and contain site characteristics (e.g., latitude / longitude, vegetation and climate classification), variable information (e.g., height / depth, instrument model), and ecological data collected at the site (e.g., canopy height, LAI, soil characteristics). New online documentation describes available BADM groups and variables (https://ameriflux.lbl.gov/data/badm/badm-standards/).

The *FLUXNET data product*, which is compatible with the FLUXNET2015 dataset, is generated with the ONEFlux processing codes that gap-fill, partition fluxes, and perform uncertainty analysis. An evaluation version of the data product is available for over 60 sites. AMP has integrated ONEFlux into the AmeriFlux data processing pipelines as described on new webpages (https://ameriflux.lbl.gov/data/data-processing-pipelines/). The production release of the FLUXNET data product for over 20 AmeriFlux sites is scheduled for September 2021.

AMP also provides data services targeted for Earth science researchers. To support the new CC-BY-4.0 license and upcoming production FLUXNET data release, we have revamped the data-related pages on the AmeriFlux website. Data users can more easily discover and select data by variables, years, data-sharing policy, data product, and site characteristics on the Site Search page. The Data Download page has been retooled to enable multiple ways to select sites' data for download. The Site Sets functionality provides a way for registered users to create groups of sites that are used regularly. Citations and Site PI information can be downloaded easily for any Site Set. Finally, a customizable mapping feature allows data users to easily create maps of sites of interest.

Title: **Expanding and Growing the ESS-DIVE Repository Community**

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BER Program: ESS

Project: DOE Lab-led project (Lawrence Berkeley National Laboratory)

Project Website: https://ess-dive.lbl.gov/, https://data.ess-dive.lbl.gov/ (repository)

Project Abstract:

The Environmental System Science - Data Infrastructure for a Virtual Environment (ESS-DIVE) serves as the repository for archiving data generated by ESS projects. The ESS-DIVE repository provides long-term stewardship and use of data from observational, experimental, and modeling activities within the DOE's Environmental System Science program (ESS). The ESS-DIVE repository is designed as a scalable framework allowing ESS data providers to contribute standardized, structured, and high-quality data that enables users to develop data processing, synthesis, and analysis capabilities using its data along with external data available from partner systems.

The ESS-DIVE project objectives are:

- Expanding data archiving across the ESS community;
- Enhancing the data package lifecycle to support cradle to grave archiving;
- Support for archiving larger datasets including model data;
- Capabilities for advanced search, discovery, access, and reuse of FAIR ESS data;
- Scalable, robust production and data preservation systems; and
- Building and supporting an engaged user community.

Title: ExaSheds: Advancing Watershed System Science using Machine Learning and Data-Intensive Extreme-Scale Simulation

Carl Steefel[1]*, Scott Painter[2], Xingyuan Chen[3], Ethan Coon[2], Dipankar Dwivedi[1], David Moulton[4], Alison Appling[5], Alexander Sun[6]

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Project Lead Principle Investigators (PI): Steefel and Painter

BER Program: Data Management

Project: ExaSheds

Project Website: https://exasheds.org

Project Abstract: The ExaSheds project is exploring synergies between data-driven machine learning (ML) approaches and process-based hydro-biogeochemical high-performance computing (HPC) simulations with the objective of improving predictive capability for watershed and river basin function. The new set of hybrid ML+HPC and ML tools are being developed to enable scientific discovery of both present-day watershed function, and also to extend predictive capability to future climate scenarios where ML-only approaches may be challenged.

The project is pursuing several research themes and applying the resulting tools in integrated demonstrations studies of watershed to basin-scale function in two study areas: the Upper Colorado Water Resources Region (UCWRR) and the Delaware River Basin (DRB).

The project is using ML to generate difficult-to-observe model inputs from sparse, coarse, and indirectly related observations. We developed an approach to sequential imputation of missing spatio-temporal precipitation data (Mital et al, 2020) and modeling the distribution of snow-water equivalent by combining precipitation and temperature with LIDAR maps (Mital et al, submitted).

The use of ML+HPC hybrid models is being explored as an alternative to traditional inverse modeling. As a preliminary step, we have developed a deep neural network (DNN)-based inverse modeling method that estimates the subsurface permeability of a watershed from stream discharge data (Cromwell et al, 2021).

We are exploring the use of hybrid ML-physics models for hydrology. We developed a hybrid streamflow model that use output of a hydrological model as one of the inputs to a Long Short-Term Memory (LSTM) network. That hybrid approach outperforms standalone LSTM on diverse catchments (Konapala et al, 2020) and when trained on short datasets (Lu et al, 2021).

We are developing a new set of reduced dimension and reduced order models for biogeochemistry. Our initial effort has focused on developing an approach for representing hillslope fluxes using an ensemble of flowtubes that is applicable to transient, variably saturated conditions.

A simulation (hydrology and geochemistry) capability on heterogeneous computer (GPU+CPU) architectures is being developed, using the DOE software Amanzi-ATS and Crunch. This is

providing vastly improved simulation throughput capacity to support model-data integration and enabling large-scale simulations on leadership class computing facilities.

References

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Mital et al, 2020. *Frontiers in Water 2: 20. doi: 10.3389/frwa*.

Cromwell et al, 2021. *Frontiers in Earth Science* 9:613011. doi: 10.3389/feart.2021.613011

Lu et al, 2021. *Journal of Hydrometeorology*, *22*(6), 1421-1438.

Title: **Parameters Controlling Ecosystem CO_2 Responses in Simulations of Duke and Oak Ridge FACE Experiments with ELM-FATES-CNP**

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Project Lead Principal Investigator (PI): Anthony Walker

BER Program: ESS

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

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

Project Abstract: The response of temperate forests to elevated atmospheric CO_2 (eCO2) is constrained by nitrogen (N) availability and dynamics, which can interact with demographic traits and processes. Understanding these interactions is necessary to develop predictive understanding of forest ecosystem responses to eCO2 at climate-change relevant timescales (i.e. decades). However, even the long-term FACE experiments such as Duke and Oak Ridge only ran for about a single decade. Results over a single decade provide some information on eCO2, N, and demographic process interactions but our ability to understand longer-term vegetation processes remains limited. Furthermore, the heterogeneity of demographic states represented by FACE experiments is also limited. The Functionally Assembled Terrestrial Ecosystem Simulator (FATES) is a model with the demographic resolution that enables us to evaluate how demographic traits and processes might interact with eCO2 over longer timescales. Recent developments to bring nutrient cycling into ELM-FATES (ELM-FATES-CNP) now provide the N and other nutrient-related constraints that are known to be an essential driver of ecosystem eCO2 responses. In this poster we apply ELM-FATES-CNP to simulating the Duke and Oak Ridge FACE experiments. We use the two soil nutrient cycling hypotheses or conceptualizations that currently exist in ELM—relative demand and equilibrium chemistry approximation. Results presented in this poster are based on initial simulations and informal sensitivity analyses to investigate and define parameter sets and provide a baseline understanding of ELM-FATES-CNP responses to eCO2. These parameter sets and understanding will be used to develop and interpret an ensemble of demographic model simulations to evaluate the question: How have demographic processes shaped the responses to eCO2 observed at long-term FACE experiments?

Title: **Accelerating Local to National Watershed Science through the IDEAS-Watersheds Software Ecosystem**

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BER Program: ESS
Project: IDEAS-Watersheds
Project Website: https://ideas-productivity.org/ideas-watersheds

Project Abstract:

Flexible workflows that enable scientists to easily integrate field and lab data with their conceptual model development and analysis are paramount to advancing our scientific understanding of watersheds. Such workflows include pre-processing of site data for model setup, parametric sensitivity analysis and parameter estimation, and subsetting of model output for use in subgrid models and analysis of model performance. The IDEAS-Watersheds open-source community driven software ecosystem provides the fundamental building blocks for these workflows as it includes workflow tools such as the pre-processing tools TINerator, PriorityFlow and Watershed Workflow, which prepare watershed data for use in models. In this poster we highlight two applications of workflow tools to hydrological modeling performed using codes in the IDEAS Watersheds software ecosystem.

First, an integrated watershed model has been developed for American River watershed (ARW) within the Yakima River Basin (YRB) by leveraging a community workflow in Jupyter notebooks that generates unstructured meshes and prepare ATS input files from multiple data sources, such as USGS NHDplus, NRCS land cover data products, USDA soil maps, and others. Long term (1997-2020) ATS model simulations have produced stream discharges at the ARW outlet that better match observations at the USGS stream discharge at the outlet than the more empirical SWAT simulations. The evapotranspiration (ET) and snow water equivalent (SWE) dynamics simulated by ATS show good agreement with MODIS ET and SWE data products. Watershed models were also developed for the Upper Colorado River Basin and the Delaware-Susquehanna Basin using the ParFlow CONUS model. We leveraged the capabilities and the new ParFlow-Python interface to subset these domains from the CONUS2.0 model. We ran ensembles of simulations across both domains testing a suite of subsurface parameterizations. We compared simulation output to USGS stream gauges and groundwater wells to evaluate

model performance across a range of hydrogeologic configurations. These test beds informed our final national scale parameters and provided a testing ground for transferable watershed workflows.

These examples highlight how flexible workflow tools enable hydrological modeling across scales as part of a software ecosystem that also includes the necessary process-based simulators.

Title: Interoperable and Reusable Software Enables Reactive Transport Modeling at Watershed Scales

Scott Painter[1]*, Sergi Molins[2]*, Dipankar Dwivedi[2], Ahmad Jan[1], Ilhan Özgen-Xian[2], Ethan Coon[1], Saubhagya Rathore[1], Daniil Svyatskiy[3], Zexuan Xu[2], David Moulton[3]

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Project: IDEAS-Watersheds
Project Website: https://ideas-productivity.org/ideas-watersheds/

Project Abstract:

Although reactive transport modeling (RTM) has a long history and proven value in advancing mechanistic understanding of hydro-biogeochemical processes at small scales, application of reactive transport models at the large spatial scales needed to advance understanding of watershed function is relatively rare. Central among the many challenges in bringing RTMs to the watershed scale are the large computational demands, the complementary roles played by surface and subsurface systems, and the multiscale nature of hydrological and biogeochemical interactions. We present examples of how the IDEAS-Watersheds project is advancing an ecosystem of interoperable and reusable software that enables modelers to meet those challenges. The integrated surface/subsurface hydrology code Amanzi-ATS [1] has been extended [2] to model fully coupled reactive transport in shallow surface waters, the vadose zone, and groundwater. A key enabling technology is the Alquimia interface [3], which makes it possible for ATS to access capabilities from existing biogeochemical reaction models. Another key capability is Amanzi-ATS's flexibility in handling multiple computational meshes and process models, which has enabled a novel multiscale model structure [4] that makes it possible to represent biogeochemical process understanding gained from laboratory or small-scale field investigations in much larger models. Watershed-scale reactive transport simulations for Copper Creek Watershed, East River, Colorado demonstrate the fully coupled integrated hydrology RTM capability, and network-scale simulations of nutrient dynamics in the Portage River Basin, Ohio demonstrate the multiscale capability. This work emphasizes the need for flexible modeling frameworks that allow for deployment of new capabilities while supporting the implementation of complementary approaches.

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[2] Molins et al., A new approach to simulate integrated-hydrology and reactive-transport modeling, In preparation.

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Soil Carbon Dynamics During Drying vs. Rewetting: Importance of Antecedent Moisture Conditions

Kaizad F. Patel,[1*] Allison Myers-Pigg,[1,2] Ben Bond-Lamberty,[3] Sarah J. Fansler,[1] Cooper G. Norris,[4] Sophia A. McKever,[1,5] Jianqiu Zheng,[1] Kenton A. Rod,[6] Vanessa L. Bailey[1]

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Project Lead Principal Investigator (PI): Vanessa L. Bailey

BER Program: Environmental System Science (ESS)
Project: Pore to Core: Linking Soil Organic Carbon Protection Mechanisms to Ecosystems CO_2 Fluxes in Response to Varying Antecedent Soil Moisture Conditions

Project Abstract:
Soil moisture influences soil carbon dynamics, including microbial growth and respiration. The response of such soil respiration to moisture changes is generally assumed to be linear and reversible, i.e., to depend only on the current moisture state. Current models thus do not account for antecedent soil moisture conditions when determining soil respiration or the available substrate pool. We conducted a laboratory incubation to determine how the antecedent conditions of drought and flood influenced soil organic matter (SOM) chemistry, bioavailability, and respiration. We sampled soils from an upland coastal forest, Beaver Creek, WA USA, and subjected them to drought (7 days) or flood (saturation) and then rewet or dried, respectively, to 5, 35, 50, 75, and 100 % saturation. We measured respiration and water extractable organic carbon (WEOC) concentrations and used ^{1}H-NMR and FT-ICR-MS to characterize the WEOC pool across the treatments. The drying vs. rewetting treatment strongly influenced SOM bioavailability, as rewet soils (with antecedent drought) had greater WEOC concentrations and respiration fluxes compared to the drying soils (with antecedent flood). In addition, air-dry soils had the highest WEOC concentrations, and the NMR-resolved peaks showed a strong contribution of protein groups in these soils. Both NMR and FT-ICR-MS analyses indicated increased contribution of complex aromatic groups/molecules in the rewet soils, compared to the drying soils. We suggest that drying introduced organic matter into the WEOC pool via desorption of aromatic molecules and/or by microbial cell lysis, and this stimulated microbial mineralization rates. Our work indicates that even short-term shifts in antecedent moisture conditions can strongly influence soil C dynamics at the core scale. The predictive uncertainties in current soil models may be reduced by a more accurate representation of soil water and C persistence that includes a mechanistic and quantitative understanding of the impact of antecedent moisture conditions.

Title: Soil Respiration Modeling and Prediction Variabilities Across Scales

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Project Lead Principal Investigator (PI): Vanessa Bailey

BER Program: ESS
Project: Pore to Core: Linking Soil Organic Carbon Protection Mechanisms to Ecosystem CO_2 Fluxes in Response to Varying Antecedent Soil Moisture Conditions

Project Abstract: Soil respiration is a major component of the global carbon cycle, and it is regulated by a multitude of biotic and abiotic factors and their interactions. Predictive models rely on both empirical data and the underlying theory to provide robust predictions, yet model simplifications are often necessary due to data and parameterization limitations. This is particularly true for modeling soil moisture-respiration relationship, given that the control water exerts on soil respiration remains challenging to capture at various scales. Here we took both bottom-up and top-down models and evaluated the scale-dependence of model simplifications. In the microscale diffusion-based bottom-up model, we derived a generalizable analytical solution of diffusion-limited nonlinear microbial uptake kinetics, in which microbial metabolic rates were governed by both physical and biological drivers via substrate diffusion and effective microbial-substrate binding. This mechanistic model accounting for soil texture-dependent microscale (~10 to 200 μm) heterogeneity accurately captured observed variations of soil moisture-respiration relationships in laboratory incubations. However, when evaluated with field observations, this mechanistic model did not show significant advantage over simplified polynomial functions. This result indicates control factors, such as soil topography, vegetation etc. that operates at field-to-site scales could be more important in explaining field based observations. In the top-down modeling, we evaluated the relationships between soil respiration and soil water content (SWC) or precipitation with a monthly global soil respiration database (MGRsD). Relationships between soil respiration and monthly soil water content or precipitation vary widely across the 507 sites encompassing a wide variety of environmental conditions. The correlation between soil respiration and SWC or precipitation drastically decreased when data from different sites were aggregated at larger scales (i.e., climate region), further supporting site-specific parametrization of soil moisture-respiration relationships. These two studies with distinct modeling approaches both identify the importance of scale aggregation in soil respiration modeling and simplification. There remains a profound gap between mechanistic models targeting soil microscale heterogeneity and data driven models focusing on regional and global patterns. Developing site-specific understanding of soil functionality that integrates the spectrum of abiotic and biotic processes is an important next step for increasing scale-awareness of current modeling practice and identifying data needs to illuminate the complexity of soil functionality across scales.

Title: **An Iterative Approach to Linking Genome Scale Metabolic Models with Reactive Transport Simulation**

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Project Lead Principal Investigator (PI): Rebecca Rubinstein

BER Program: SBIR/STTR

Project: Other Institution project

Project Website:

Project Abstract:

Critical zone hydrobiogeochemical systems play a key role in carbon and water cycling, which makes them extremely important both scientifically and economically. The “bio” component of these systems is known to drive many core processes, but is often treated as a black box when integrated with large scale simulations due to the challenge of linking across domains and scales. As a result, these simulations may fail to capture complex interactions between the critical zone microbial community and the surrounding environment. We have previously demonstrated a means by which genome scale metabolic models built in KBase may be used to inform PFLOTRAN reactive transport simulations in order to better define the chemistry of microbe-driven reactions. Flux balance analysis performed in KBase is used to describe the reaction stoichiometry used in PFLOTRAN, so the reactions are based on actual microbial metabolisms rather than rule-of-thumb approximations. We now expand this approach to include iteration between the metabolic and reactive transport models so that the two components evolve alongside and in response to one another. Thus, we can predict how the system will behave over time as limiting resources change and various nutrients are exhausted or newly created. For demonstration purposes, we have applied this approach to nitrogen cycling in hyporheic zone sediments. The initial model definition is based on real-world samples collected from Hanford 300 reach sediments. This includes a simplified microbial system based on metagenomic analysis and chemistry defined based on geochemical and metabolomics analysis. With each iteration, the chemical profile simulated using PFLOTRAN is provided to KBase as a new media formulation and used to generate new flux balance analysis solutions, which then in turn provide new stoichiometries for the microbe-driven reactions. This approach allows our simulations to better capture ongoing system dynamics as well as short-term responses to perturbations.

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

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BER Program: ESS

Project: Argonne Wetland Hydrobiogeochemistry SFA

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

Project Abstract: Within wetlands, movement of water and biogeochemically catalyzed transformations of its constituents determine the mobility of nutrients and contaminants, emission of greenhouse gasses into the atmosphere, carbon (C) cycling, and the quality of water itself. The long-term objective of the Argonne *Wetland Hydrobiogeochemistry* Scientific Focus Area (SFA) is the *development of a mechanistic understanding and ability to model the coupled hydrological, geochemical, and biological processes controlling water quality in wetlands and the implications of these processes for watersheds commonly found in humid regions of the*

United States. To accomplish this, the Argonne *Wetland Hydrobiogeochemistry* SFA focuses research on a riparian wetland within Tims Branch at the Savannah River Site. Tims Branch contains riparian wetlands representative of those commonly found in humid regions of the Southeast that have C-rich soils and high Fe content. However, it is unique in that parts of the watershed received large amounts of contaminant metals and uranium as a result of previous industrial-scale manufacturing of nuclear fuel and target assemblies. 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 hypothesis of our research is that *hydrologically driven biogeochemical processes that create redox dynamic conditions from the nanometer to meter scales are a major driver of groundwater and surface water quality within riparian wetland environments*.

We identified three major components (focus areas) of the Tims Branch riparian wetland that represent critical zones containing hydrologically driven biogeochemical drivers, which control water quality: *sediment, rhizosphere, and stream*. Within these three focus areas, we identified two common thematic knowledge gaps that inhibit our ability to predict controls on water quality:

(1) In-depth understanding of the <u>molecular-scale biogeochemical processes</u> 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 <u>mass transfer</u> 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 hydrobiogeochemical conceptual model of the Tims Branch riparian wetland.

Hydrobiogeochemical Processes Impacting Uranium Speciation and Transport in Tims Branch, Savannah River Site

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BER Program: SBR

Project: Argonne Wetland Hydrobiogeochemistry SFA

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

Project Abstract: The Argonne *Wetland Hydrobiogeochemistry* SFA studies are centered on a riparian wetland field site within Tims Branch at the Savannah River Site. As for many wetland environments, wetlands within Tims Branch are subject to both seasonal and episodic changes in hydrologic conditions affecting the degree of saturation, and thereby the redox state, of soils and sediments. The redox dynamic nature of these soils/sediments is driven largely by microbial activity that results in active biogeochemical cycling of major elements (i.e., Fe and S) as well as trace metals including U. Synchrotron x-ray spectroscopic measurements of sediment cores collected within the wetlands show a strong correlation between the degree of saturation and the redox state, as indicated by the valence of Fe and U, with Fe(III) and U(VI) predominant in unsaturated sediments and Fe(II) and U(IV) in saturated sediments. U(IV) in the saturated sediments is present as mononuclear U(IV) ions, that readily oxidize to U(VI) on exposure to air. The redox dynamic nature of the wetlands is also illustrated by the formation of iron-enriched flocs along gaining sections of Tims Branch, where anoxic groundwater containing Fe(II) contacts oxygenated overlying water. The flocs contain Fe (9.7% on a dry mass basis)—in the form of ferrihydrite (83% of Fe) and lepidocrocite (17%) as determined by Fe K-edge EXAFS spectroscopy—as well as P (2.7%), S (1.2%), and Al (0.4%). The flocs are effective scavengers of U, with concentrations ranging from < 0.05 ppm in uncontaminated areas to as high as 600 ppm in the contaminated area, depending on location. Furthermore, the concentration of U within the flocs was found to vary by an order of magnitude in response changes in streamflow due to episodic rain events, suggesting the potential importance of flocs in controlling U transport at the site. The stability of flocs varies over time and they can undergo microbially mediated cycling of

redox active elements such as Fe and S, the effects of which on U speciation within the flocs in situ is as yet unknown, as is the fate of U when the flocs degrade/disperse; however, preliminary microcosm studies indicate that floc-associated U(VI) is reduced to U(IV) when flocs are exposed to anoxic conditions.

Molecular to Core-Scale Biogeochemistry at Tims Branch Wetland, Savannah River Site

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BER Program: SBR

Project: Argonne Wetland Hydrobiogeochemistry SFA

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

Project Abstract: The Argonne SFA project (*Wetland Hydrobiogeochemistry*) studies the processes that govern elemental cycling and particle formation/transport at the oxic-anoxic interfaces of a DOE field site, the Tims Branch wetlands at Savannah River National Laboratory. The variable redox nature of this riparian ecosystem creates conditions for the formation and dissolution of iron mineralization products, which can influence carbon and phosphorous balances, as well as the mobility of contaminants discharged during past operations (Ni, Cr, Zn, Pb, and U). Recognizing the potential value of using U as a sentinel for sediment redox state and particle-associated transport, the distribution of uranium along Tims Branch was mapped on the kilometer and meter scale using helicopter- and backpack-borne gamma detectors. Results show that 83% of the contamination released in the 1970s remains in the wetland and that the contamination accumulated in limited portions along the wetland where the stream had broadened and flow was slow. These results at the watershed scale not only quantify the longevity of contaminant sequestration, but also provide an idea of the hydrological as well as the biogeochemical factors responsible for sequestering elements/particles in riparian wetlands. To understand the influence of pore-scale wetland conditions on the molecular speciation of Fe and U, specific locations on the radiation maps were chosen for sediment coring. The elemental content and speciation with depth was determined in the intact cores at millimeter resolution by synchrotron x-ray spectroscopy. U accumulated in the top 5-10 cm of the sediment and correlated with Fe and the other contaminants, suggesting that the distribution was due to particle

deposition rather than precipitation from groundwater. The valence of U varied with depth and coring location, predominating as U(IV) in saturated sediments and as U(VI) in drier locations. Reduced U correlated with reduced Fe species and an increase in fermentative and metal-cycling bacteria, as well as with O_2 profiles observed at the site. U EXAFS spectroscopy revealed that the reduced U species are mononuclear U(IV) ions, rather than the UO_2 species predicted by models. To elucidate the speciation, we studied controlled systems with U(IV) bound to minerals and organic ligands (citrate, EDTA). The spectral comparisons suggested that sediment-associated U(IV) was bound to mineral surfaces. Our multiple-scale characterization results indicate a previously unappreciated importance of U(IV) species and particle transport at the site, which together with the observed redox variability over a few centimeters presents a challenge for modelling elemental speciation and transport.

Soil Carbon Response to Environmental Change – Argonne Soil Dynamics SFA Overview

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

Project Abstract: The Argonne Scientific Focus Area (SFA) on soil dynamics conducts fundamental research to quantify and characterize soil carbon stocks, evaluate their potential responses to environmental change, and develop data products that can inform model development. We envision our role in the DOE integrated model-observation-experiment paradigm (ModEx) as translating an understanding of the processes and mechanisms driving the distribution, composition, and dynamics of soil organic carbon stocks into (1) informed collection of new observations, (2) characterization of soil organic matter (SOM) pools and factors affecting their dynamics and persistence, and (3) development of products to benchmark, constrain, and validate process models at multiple scales.

At present, research focuses on soils of the northern circumpolar permafrost region, where climatic changes are causing widespread permafrost thawing, hydrologic changes, and related disturbances that are accelerating SOM decomposition rates and increasing greenhouse gas emissions from one of Earth's largest organic carbon reserves. Current SFA objectives are (1) provide reliable assessments of the spatial and vertical distributions of soil carbon stocks in permafrost regions, and (2) develop empirical tools for predicting the potential decomposability of carbon stored in permafrost region soils. Our approach to these objectives integrates focused field campaigns and new sample collection, archived soil resources, laboratory/spectroscopic analytical tools, and geospatial modeling. To reduce observational uncertainties caused by the unique cryo-pedogenic processes occurring across permafrost-affected landscapes, our field campaigns are targeting how soil carbon distributions are influenced by development of ice-wedge polygons on lowland coastal plains, topographic position within hillslope landscapes, and formation of river deltas. To evaluate the relationships between the composition and potential decomposability of SOM pools preserved in permafrost-region soils, we are coupling physical/chemical fractionation and spectroscopic approaches with standardized incubation bioassays. Multivariate calibration models are being developed to predict these laboratory measurements from the mid infrared (MIR) spectra of bulk soils representing different circumpolar soil types and ecoregions. Ultimately, the calibration models will be applied to the MIR spectral library we are building for soils collected by the SFA and its collaborators from across the northern circumpolar region to enable widespread geospatial interpolation and assessments of SOM composition and potential decomposability at landscape to regional scales.

Quantifying and Representing Variability in Permafrost-Affected Soils across Ice Wedge Polygons for Improved Sampling Strategies, Prediction, and Modeling

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BER Program: ESS

Project: Argonne National Laboratory Soil Dynamics SFA

Project Website: https://ess.science.energy.gov/anl-sfa/ and http://tessfa.evs.anl.gov/

Project Abstract: Efforts to bridge scaling gaps when extrapolating soil properties and carbon stocks from soil profiles to sites and landscapes are significantly challenged by the highly heterogeneous nature of permafrost-affected soils. In many areas of the northern circumpolar region, this fine-scale heterogeneity is associated with patterned ground features such as ice wedge polygons (IWPs), non-sorted circles, stripes, and earth hummocks. Upscaling heterogeneous point data to the scale of individual sites or patterned ground features in permafrost regions without loss of information requires conducting data synthesis while also retaining uncertainty estimates. Efforts to overcome these challenges have ranged from generating two-dimensional representations of soils across patterned ground features to intensive, core-based one-dimensional sampling at fine scales. Two-dimensional representations of soil profiles across patterned ground features have the advantage of allowing for more accurate spatial and vertical characterization by accounting for the area of each soil horizon or layer within each incremental horizontal or vertical slice of interest within the profile. Utilizing data from soils sampled across flat-centered, low-centered, and high-centered IWPs near Utqiaġvik, Alaska, we demonstrate how exploring and synthesizing variability at multiple scales can inform sampling strategies and best practices for soil carbon stock estimation using rapid, core-based methods. Beginning with two-dimensional representations of soil variability across full IWPs, we generate populations of carbon stocks and down-profile patterns of other soil constituents (ice, total nitrogen, bulk density) across individual polygon components (such as ice wedge troughs vs. polygon centers) by pseudo-sampling these two-dimensional representations using digital workflows. The results of our analysis show how bridging these scaling gaps can lead to improved, rapid, data-driven sampling strategies for carbon stock estimation of IWPs, which can reasonably approximate mean carbon stocks of entire IWPs or carbon stocks for individual spatially scalable components of IWPs.

Understanding Composition and Decomposability of Arctic Soils by Integrating Laboratory Incubations with Spectroscopy Measurements and Models

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BER Program: ESS

Project: Argonne National Laboratory Soil Dynamics SFA

Project Website: https://ess.science.energy.gov/anl-sfa/ and http://tessfa.evs.anl.gov/

Project Abstract: In the permafrost region, the relative importance of mechanisms affecting soil organic carbon (SOC) mineralization rates differ from those of other ecoregions. Thus, the composition and potential decomposability of soil organic matter (SOM) are key uncertainties in models projecting the amount of SOC that might be released to the atmosphere from this region. In past studies, we demonstrated that the mid-infrared (MIR) spectra of bulk soils are sensitive to the degradation state of SOM and can predict short-term carbon mineralization from arctic tundra soils. Here, we explore the decomposability of soils collected from ice-wedge polygons formed on glaciomarine sediments near Utqiaġvik, Alaska. The soils were incubated aerobically at 15°C and 5°C for more than two years, and CO_2 production was measured periodically and modeled. Soil physicochemical properties including particle density, total organic carbon, total nitrogen, and SOM composition were also determined. We derived very good partial least square regression (PLSR) models of cumulative CO_2 production (expressed on the basis of soil mass) from the MIR spectra of these soils. Analysis of the beta coefficients for the PLSR models suggest that the amounts of clay minerals, silicates, and the organic functional groups indicative of aliphatics and polysaccharides were the primary drivers of differences in SOC mineralization. Although the cross validation PLSR models had R^2 values ranging from 0.93 to 089 for incubation periods of 6 to 24 months, the PLSR models tended to underestimate CO_2 production after 6 months. Thus, we are currently evaluating whether other chemometric or machine learning algorithms can improve predictions of long-term mineralization. Nevertheless, the overall success of the PLSR models demonstrates the predictive potential of MIR spectra, which is derived from the ability of this analytical tool to integrate information on the amounts of both SOC and soil minerals, as well as the types of organic compounds in each soil. The ultimate goal of our research is to link geo-referenced estimates of SOM composition and potential decomposability with environmental co-variates to create geospatial assessments and maps, which can serve as benchmarks for process models at landscape, regional, and global scales.

Coastal Observations, Mechanisms, and Predictions Across Systems and Scales – Field, Measurements, and Experiments (COMPASS-FME)

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

Project Abstract: Coastal terrestrial-aquatic interfaces (TAIs) occupy relatively small areas of the Earth's surface but play an outsized role in global biogeochemical cycles. Both marine and freshwater coastal TAIs compress and expand with tides, sea- and lake-level variation, global change, and land use, making prediction of C and nutrient dynamics difficult.

The Coastal Observations, Mechanisms, and Predictions Across Systems and Scales – Field, Measurements, and Experiments (COMPASS-FME) pilot study is a multi-institutional effort to understand the interactions of waters, soils, microbes, and plants within coastal TAIs to inform the development, testing, and application of multiscale, hierarchical models. COMPASS is being piloted at select sites in the Chesapeake Bay and Lake Erie regions to understand the causes, mechanisms, and consequences of the shift between aerobic and anaerobic conditions related to the interacting water-soil-microbe-vegetation system. We focus on the fluxes and transformations of carbon, nutrients, and redox-sensitive elements in ecosystems influenced by coastal water exchange; these gaseous, aqueous, and particulate fluxes and transformations must be mechanistically resolved to enable coupling between land, wetland, and open-water systems in regional models and ultimately Earth system models. Studies in these two regions allow us to compare and contrast how ecosystem control points emerge along differing gradients in topography, soil saturation, ionic strength, redox state, and nutrient availability.

Our research is guided by model analyses and benchmarking to identify model uncertainties and sensitivities and data syntheses to prioritize measurement needs. We leverage ongoing, multi-agency studies to gather consistent data from dozens of locations and capture temporal dynamics with synoptic studies in multiple fixed and temporary locations. Experiments will test hypotheses about the interactions among waters, soils, microbes, and vegetation at coastal TAIs. This plan addresses a DOE priority for a systems-level understanding of coastal ecosystems that integrates measurements, models, and experiments to develop a scalable, flexible, and process-rich coastal ecosystem modeling framework.

Gaining a predictive understanding of coastal ecosystem responses to press and pulse hydrologic disturbance

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Project Lead Principal Investigator (PI): Vanessa Bailey

BER Program: ESS
Project: COMPASS
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Project Abstract: Coastal ecosystems are undergoing dramatic changes as sea-level rise (SLR) accelerates and precipitation and storm regimes change. SLR gradually exposes coastal landscapes to seawater (press disturbance) and increasing storm frequency and magnitude leads to acute seawater and freshwater saturation events (pulse disturbance). We implemented two manipulative, ecosystem-scale field experiments to understand and predict the influence of press and pulse disturbances on coastal ecosystems. The first investigated the initial (2-y) responses of soil C cycling and chemistry to novel hydrologic disturbances by transplanting soil monoliths between sites varying in natural salinity and inundation regimes (press). Coastal soil carbon dioxide (CO_2) flux, but not methane (CH_4) flux, was affected by changing hydrologic regimes; responses were dependent upon the salinity and inundation legacies of the monolith's original location. Soils with a history of exposure to salinity and inundation were resilient to novel disturbances, with CO_2 emissions increasing with rising salinity. Conversely, soils that lacked such legacies were vulnerable to shifting hydrologic conditions and soil respiration was suppressed. We propose that hydrologic legacies promoted the persistence of resilient, salt-tolerant microorganisms that were able to use increased resource availability (nutrients, electron acceptors) following seawater exposure. Lack of such legacies likely led to microbial communities that were sensitive to osmotic and redox stress following seawater exposure. Our second experiment – TEMPEST (Terrestrial Ecosystem Manipulation to Probe the Effects of Storm Treatments) – simulates ecosystem-scale freshwater and seawater soil saturation events in a well-drained, coastal upland forest (pulse). Our goal is to understand the initial and cumulative effects of soil saturation on deciduous upland forests. The experiment uses a large-unit (2,000 m^2), un-replicated experimental design, with control, freshwater, and seawater soil saturation treatment plots. Treatment plots will receive 300 m^3 of fresh- or seawater, saturating the soil to 30 cm for 10 hours. Treatment frequency will increase over a decade to identify tipping points where plant and microbial communities and biogeochemical cycles begin to change rapidly. Pre-treatment data collection began in 2019 and the first full simulation is scheduled for June 2022. This experiment provides us with an unparalleled opportunity to disentangle the effects of saturation and salinity under in-situ conditions and at an ecosystem-scale.

COMPASS-FME: Early Successes in Data Synthesis and Modeling Analysis

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Project Lead Principal Investigator (PI): Vanessa Bailey
BER Program: ESS
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Project Abstract:
Tight coupling of models, model-derived hypotheses, observations, and experimentation is central to the COMPASS-FME approach to improving predictive understanding of coastal TAI processes. We designed and carried out a set of focused data syntheses, model analyses, uncertainty quantification exercises, and sensitivity analyses to inform where, when, and how to carry out early observation and experimentation elements of COMPASS-FME. These initial activities also helped us to clarify which process representations are lacking within current modeling frameworks, and at which spatial scales new process representations might need to be included to improve system-level prediction.

Our data synthesis work focused on areas in which models such as ELM-PFLOTRAN (used in a number of COMPASS-FME activities) tend to have prediction difficulties. These include (i) understanding how top-of-column CO2 flux is affected by changes in water availability and drainage; (ii) examining how seawater inundation alters vegetation dynamics, and the mechanisms driving these changes; (iii) quantifying water biogeochemistry and quality variation through time and space in the COMPASS-FME domain; and (iv) probing the degree to which coastal marsh plant production is driven by growing season phenology, tidal flooding, and species-specific effects. A final 'functional zonation' task focuses on spatial synthesis and inference and will be used to scale results and models across the project.

In the area of modeling analyses, we carried out two studies using the ELM-PFLOTRAN framework to quantify modeling uncertainty and parameter sensitivity for new representation of coastal wetland vegetation types, and subsurface biogeochemical processes. We used a coupled modeling approach that integrated vegetation, soil, microbial processes, and hydrology within the coastal TAI. We learned that both C3 and C4 plant types are both important to overall predictions, but that the vegetation parameterizations for the C4 types need greater focus to reduce uncertainty. We also identified a suite of vegetation processes which should be prioritized for further study, including controls on leaf phenology, controls on plant respiration, rates of mortality, and parameters influencing the decomposability of soil organic matter. Results from our modeling investigation of subsurface biogeochemistry showed that the redox dynamics of the coastal wetland sites can be captured reasonably well, and highlighted some new measurements that should be included at the COMPASS-FME sites.

Biogeochemical Transformations at Critical Interfaces in a Mercury Perturbed Watershed Science Focus Area

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BER Program: Environmental Systems Science

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: Freshwater resources supplied by headwater streams and their surrounding watersheds are being threatened by severe pollution from anthropogenic releases of nutrients and trace metals (e.g., mercury [Hg]). Preserving these services for future use requires developing a deeper understanding of watershed structure and function. Research findings during Phase I of the Critical Interfaces Science Focus Area (SFA) project have led to the realization that transient storage zones (TSZs), and more specifically metabolically active TSZs (MATSZs) are important locations for further investigation. While TSZs are surface and subsurface locations (e.g., hyporheic zone) that delay the downstream flow of water in comparison to the main channel; MATSZs are associated with the interstitial spaces of hyporheic zone streambed that are microbially active and pore space present in the microbiome of in-stream biofilm. Unlike TSZs, MATSZs exhibit very different biogeochemical environments (e.g., redox conditions) compared with the flowing stream or streambed, making them important "hot spots" that account for a substantial proportion of the diverse and intensified biogeochemical activity in watersheds.

The SFA is progressively advancing our understanding of the factors that influence watershed structure and function using Hg and the East Fork Poplar Creek (EFPC) watershed as representative use cases. The EFPC watershed offers a unique niche to the ESS program by being nested in the most intensively used freshwater Water Resource Region in the contiguous United States (Tennessee River Basin) and serving as a representative low-order freshwater stream system with relevance to the largest proportion of the total stream length in United States.

In FY21, the team (1) added new capabilities to the Advanced Terrestrial Simulator (ATS) modeling software creating tools that extend the model from conservative tracers to multicomponent reactive transport, (2) refined our Transient Availability Model (TAM) to include Monod-type kinetics for methylation and demethylation, (3) examined how nutrient amendments (nitrate and/or phosphate) altered stream periphyton community structure and function, and (4) continued to explore the transcriptional regulation of methylation genes under different conditions. We also advance our understanding of metal-ligand interactions that influence Hg isotope exchange and control, at a molecular scale, how methanobactin from *Methylocystis sp*. strain SB2 interacts with group 12 metals. Collectively, the aforementioned activities are providing a deeper understanding of Hg transformations in EFPC and allowing us to gain the process knowledge needed to improve predictions of carbon, nutrients, and trace metal cycling at the scale of individual stream reaches and small watershed catchments.

Changing Nutrient Concentration Alters Periphyton Biofilm Composition and Function

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BER Program: Environmental System Science

Project: Oak Ridge National Laboratory Critical Interfaces Science Focus Area

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Project Abstract: Periphyton biofilms are complex assemblages comprising algae, bacteria, fungi, detritus, extracellular polymers, invertebrates, and mineral particles. These biofilms play a central role in stream ecohydrology as they both produce (e.g., dissolved oxygen, labile carbon) and consume (e.g., nitrate, phosphate) nutrients critical to the ecosystem. They are also the site of steep geochemical gradients with conditions transitioning from fully oxic to anoxic over distances of 100 µm or less. The microbially-catalyzed production of monomethylmercury (MMHg) from inorganic mercury (Hg) is an anaerobic process. Controlled laboratory experiments have demonstrated that actively photosynthesizing biofilms may generate a significant fraction of the MMHg flux in East Fork Poplar Creek (EFPC), a Hg contaminated creek in Oak Ridge, TN.

To better understand the relationship between stream nutrient status and periphyton biofilm composition and function, we are conducting both in-stream experiments and controlled artificial stream experiments in which nutrient levels (nitrate and/or phosphate) are manipulated. The resulting biofilms are then used in experiments to quantify function (Hg methylation and MMHg demethylation kinetics) and composition (16s, 18s, ITS, and *hgcA* sequencing). Biofilms supplemented with additional nitrate and/or phosphate had lower bacterial/archaeal richness than controls in summer and higher richness in autumn. In contrast, fungal diversity in nutrient amended samples generally increased in summer and decreased in autumn relative to controls. Surprisingly, Hg methylation potential correlated with numerous bacterial families that do not contain *hgcAB*, the two-gene cluster encoding for Hg methylation ability, suggesting that overall microbiome structure of periphyton communities influence rates of Hg transformation. Microbial network analysis revealed that the nitrate amended biofilms had the highest number of hub taxa that also corresponded with enhanced Hg-methylation potential. This work provides insight into community interactions within the periphyton microbiome that may contribute to Hg cycling and will inform future research which will focus on establishing mixed microbial consortia to uncover mechanisms driving shifts in Hg cycling within periphyton habitats.

Additional experiments and development work on our transient availability model (TAM), developed for quantifying Hg methylation kinetics in biofilms, show that the TAM can be applied to describe Hg-methylation in sediments. Additionally, including expressions that

account for variable microbial activity improves model accuracy. Application of Bayesian parameter estimation methods identified model structural uncertainty and improved overall model performance.

Assessing Biogeographic Survey Gaps in Bacterial Diversity Knowledge: A Global Synthesis of Freshwaters

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Project Abstract: Organismal and genetic diversity within ecosystems is important for the mediation of ecosystem processes such as carbon and nutrient cycling, climate regulation, and ecosystem provisioning. Therefore, characterizing this biodiversity is essential for predicting and mitigating the impacts of environmental change on valued ecosystem services. Biodiversity of microorganisms is especially important given the role they serve in cycling carbon, nutrients, and trace metals within terrestrial and aquatic ecosystems and supporting plant growth and productivity. While national and global biodiversity assessments have been conducted for terrestrial vertebrates, plants, and freshwater fishes, the cataloguing of microbial diversity has been limited because technologies for describing microbial diversity have only recently become available and microbial distributions have been viewed as ubiquitous and of low conservation need. New studies have indicated microbial taxa probably exhibit biogeographic patterns, thus more detailed characterization of these communities is necessary.

In this study, we identified gaps in microbial data coverage along climatic and landscape disturbance gradients and among terrestrial biomes and hydrographic regions for all freshwater ecosystems and three freshwater habitat types: lakes and reservoirs (lentic); streams and rivers (lotic); and wetlands. Freshwaters account for <1% of Earth's surface area, yet support >10% of known plant and animal species making them disproportionately biodiverse and important ecosystems to characterize. We reviewed literature on microbial diversity in freshwaters surveyed using 16S ribosomal RNA sequencing which identify microbial taxa. We georeferenced survey locations and used a geographic information system to identify and map gaps in survey coverage using open-source data for climate, landscape disturbance, terrestrial biomes, and freshwater ecoregions. We compiled 3,425 georeferenced survey locations reported from 963 studies. Our assessment revealed high climatic coverage of freshwater microbial diversity knowledge, but expansive ecoregional gaps attributable to biased sampling near research institutions in North America, western Europe, and China. Future surveys should target ecoregions in Africa, South America, Central Asia, Australia, and Antarctica. An essential next step will be to curate and disseminate sequencing efforts to facilitate the study of processes driving global diversity patterns.

Characterization of Methanobactin Interactions with Group 11 and 12 Transition Metals

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BER Program: Environmental System Science

Project: Oak Ridge National Laboratory Critical Interfaces Science Focus Area

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Project Abstract: Methanotrophic bacteria catalyze the aerobic oxidation of methane to methanol using enzymes with copper (Cu)-based active sites. To facilitate the acquisition of Cu ions some methanotrophic bacteria secrete small post-translationally modified peptides known as methanobactins. Analogous to siderophores and iron, methanobactins strongly bind Cu ions and functions as an extracellular Cu recruitment relay. In addition to binding Cu, methanobactins will bind most transition metals and post-transition metals and protect the host methanotroph as well as other bacteria from metal toxicity. Investigating the mechanisms of methanobactin-metal interactions is essential for understanding chemical speciation, competitive interactions and biological processes involved in metal transformations. Methanotrophic bacteria are typically found at oxic-anoxic interfaces in wetlands, soils and aquatic systems and thus may have significant influence on the biogeochemical cycling of mercury and other metals. We characterized the interactions of methanobactin from *Methylocystis sp*. SB2 (mb-SB2) with transition metals using UV-Vis absorbance, fluorescence, extended X-ray absorption fine structure spectroscopy (EXAFS), and isothermal titration calorimetry, complemented by time-dependent density functional theory (TD-DFT) calculations. The metal binding site in mb-SB2 is comprised of two enethiolate groups, each conjugated with nitrogen-containing heterocycles, which facilitate interactions with a wide range of transition metal ions. The complexation of metal ions is reflected in the electronic structure of the conjugated system. Our spectroscopic data shows that mb-SB2-metal complexes may assume a range of intra- and intermolecular configurations that are distinct for each metal and depend on the metal to methanobactin ratio. We further report time-dependent changes in sample absorbance and fluorescence spectra, which occur on a wide range of experimental timescales. EXAFS data and TD-DFT calculations are consistent with tetrahedral coordination for Zn^{2+}, Cd^{2+} and linear coordination for Hg^{2+}. Furthermore, we propose a mechanism of complexation-hindered isomerization for a fluorescence enhancement observed upon the interaction of methanobactins with transition metals. This work represents the first combined computational and experimental spectroscopy study of methanobactins complexes with transition metals. Our results suggest that the methanobactins may influence the speciation and biogeochemical cycling of group 11 and 12 transition metals.

Rates and Dynamics of Mercury Isotope Exchange Reactions and Implications for Environmental Tracer Studies

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

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

Project Abstract: Enriched mercury (Hg) stable isotopes have been widely used as tracers in field and laboratory investigations of Hg biogeochemical transformations such as methylation and demethylation. Few studies, however, have considered concurrent isotope exchange reactions between newly spiked and pre-existing ambient Hg in environmental matrices. In this work, we describe detailed studies of isotope exchange reactions between spiked divalent ^{198}Hg(II) and ambient Hg(II), as well as between dissolved elemental ^{202}Hg(0)$_{aq}$ and Hg(II) bound to various environmental matrices, such as low-molecular-weight thiols, minerals, and dissolved organic matter (DOM) in water. The impact of isotope exchange on methylmercury production in the presence of organic ligands was also evaluated with an iron-reducing bacterium *Geobacter sulfurreducens* PCA (PCA). Surprisingly, we found that the spiked ^{198}Hg(II) rapidly exchanged with ligand- or mineral-bound ambient Hg(II), resulting in redistribution of Hg isotopes bound to the ligands or minerals and an apparently similar methylation rate and magnitude of the spiked Hg and ambient Hg by PCA cells. Similarly, rapid, spontaneous isotope exchange (<1 h) was observed between dissolved elemental ^{202}Hg(0)$_{aq}$ and ^{201}Hg(II)-bound to organic and inorganic ligands with varying chemical structures and binding affinities, including chloride (Cl^-), ethylenediaminetetraacetate (EDTA), cysteine, glutathione, and 2,3-dimercaptopropanesulfonic acid. Without external reductants or oxidants, the exchange resulted in transfers of two electrons and redistribution of Hg isotopes bound to the ligand but no net changes of chemical species in the system. However, an increase in the thiol-to-Hg(II) ratio decreased the exchange rates due to the formation of 2:1 or higher thiol:Hg(II) chelated complexes, but had no effects on exchange rates with ^{201}Hg(II) bound to weaker ligands, such as EDTA or Cl^-. The exchange between ^{202}Hg(0)$_{aq}$ and ^{201}Hg(II)-bound to DOM showed an initially rapid followed by a slower exchange rate due to Hg(II) complexation with both low- and high-affinity binding functional groups on DOM (e.g., carboxylates vs bidentate thiolates). Our results underscore the importance of considering isotope exchange reactions when an enriched Hg isotope is applied in environmental matrices, as the exchange could potentially lead to biased rate calculations of Hg transformation and bioaccumulation and thus risk assessments of new Hg input to the natural ecosystems.

Title: **Investigating Bedrock Groundwater Recharge Dynamics in Mountainous Watersheds**

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Project Lead Principal Investigator (PI): William "Payton" Gardner

BER Program: ESS

Project: DOE EPSCOR – University – National Laboratory Collaboration

Project Abstract:

We are investigating the effect of orographic micrometerology and shallow soil flow on deep bedrock groundwater recharge and discharge in upland catchments, to determine the dominant physical processes controlling their interaction in space and time. Accurate estimates of current and future water budgets will require knowledge of the relative volume water in surface, soil and deep groundwater, and their connections within a watershed. By far, the least understood reservoir in upland catchments is the deep groundwater system, which is complicated by high slope angles and complex topography and geology. We are measuring hydrologic connection of soil and deep groundwater with coupled shallow soil (<2 m) and deep groundwater (> 5 m) well nests on upland hill slopes, installed across a variety of landscape positions and climatic regimes, in watersheds dominated by differing lithology in northwestern Montana. Soil moisture, saturated water level, temperature and conductivity are monitored in soil and groundwater wells. Chemical and isotopic signatures are being collected and will be used to constrain fluid flux, age and provenance. Relationships between recharge flux, landscape position, local micro-climate, bedrock and soil material properties are being interpreted using our field datasets along with full Richards' equation numerical modeling of hillslope flow and transport. *We hypothesize that fundamental relationships between local climate, topography, landscape position, soil and bedrock properties exist that describe the location and amount of bedrock recharge and discharge in upland catchments*, and that by measuring these variables as well as soil and bedrock connection across a broad range of climatic, topographic and lithologic characteristics we can derive relationships which are broadly transferable to other systems. We are looking to expand the geographic and spatial scale of our sampling and data integration and interpretation methods in order to extend the range of applicability, by comparing our Montana watershed results with those of the Watershed Function Science Focus Area in the East River watershed, Colorado.

The Berkeley Lab Belowground Biogeochemistry SFA: Overview and Results of Five Years of Deep Soil Warming

Margaret S. Torn[1*], Eoin Brodie[1], Peter Nico[1], Bill J. Riley[1], Cristina Castanha[1], Rachel C. Porras[1], Jennifer L. Soong[1,2], Nicholas O.E. Ofiti[3], Michael W.I. Schmidt[3], Cyrill U. Zosso[3], Mike Rowley[1], and Ricardo E. Alves[1]

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BER Program: TES
Project: Belowground Biogeochemistry SFA (lead: LBNL)
Project Websites:
https://eesa.lbl.gov/projects/terrestrial-ecosystem-science/
https://tes.lbl.gov/

Project Abstract:
In the Berkeley Lab Terrestrial Ecosystem Science SFA, we research the role of soils in terrestrial biogeochemistry and the Earth system. Our goals are to improve process-level understanding of ecosystem-climate interactions and to develop predictive capacity suitable for Earth system models. SFA research integrates field, laboratory, and model experiments to characterize how biotic and abiotic processes influence soil carbon cycling, and may shape ecosystem responses to a warming climate. We are warming the whole soil profile to +4ºC in a well-drained coniferous forest (Blodgett Forest), and are setting up a second deep-soil warming experiment in a coastal grassland (Point Reyes). At each site, we are studying the influence of soil depth, mineralogy, biota, and climate on soil carbon dynamics. We are using results from field and lab studies to guide model development in a framework for Biogeochemical Transport and Reactions (BeTR), for the DOE E3SM land model and others.

In the first two years of the Blodgett forest warming experiment, soil respiration increased by 35% from all depths (Hicks Pries et al. 2018). After five years of warming, there is no significant attenuation trend; there is still a sustained, 30% increase in soil CO_2 efflux due to increased production throughout the soil profile (Soong et al. 2021). Moreover, subsoil (below 20 cm) carbon stocks were 33% lower in heated plots. This loss of subsoil carbon was primarily from unprotected particulate organic matter. The observed decline in subsoil carbon stocks is evidence for a positive carbon-climate feedback, which could not be concluded based on increases in CO_2 efflux alone. The high sensitivity of subsoil carbon, and the different responses of soil organic matter pools, suggest that models must capture these heterogeneous soil dynamics to accurately predict future feedbacks to warming.

Additional posters will present research on Blodgett microbiology (presented by Alves) and Point Reyes site characterization and experimental design (presented by Pegoraro and Rowley).

Publications

Hicks Pries, Castanha, Porras, and Torn. 2017. The whole soil carbon flux in response to warming. *Science* DOI: 10.1126/science.aal1319

Soong, Castanha, Hicks Pries, Ofiti, Porras, Riley, Schmidt, and Torn. 2021. Five years of whole-soil warming led to loss of subsoil carbon stocks and increased CO2 efflux. *Science Advances*, DOI: 10.1126/sciadv.abd1343

Title: Integrated Site Characterization for a New Whole-Soil Warming Experiment in a California Grassland

Elaine Pegoraro[1*], Michael Rowley[1*], Baptiste Dafflon[1], Yuxin Wu[1], Eoin L. Brodie[1], Cristina Castanha[1], Ricardo J.E. Alves[1], Nicola Falco, Jasquelin Pena[1,2], Peter Nico[1], Margaret S. Torn[1]

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Project Lead Principal Investigator (PI): Margaret S. Torn

BER Program: ESS

Project: Belowground Biogeochemistry SFA (lead: LBNL)

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

Project Abstract:

The LBNL Belowground Biogeochemistry SFA is establishing a whole-soil warming experiment in a coastal California grassland. The objective of this study was to characterize soil physico-chemical properties and seasonal hydrological dynamics along the Point Reyes warming experiment catena and vertical soil profile.

To temporally and spatially characterize the site we used remotely sensed measurements of plant properties and topography, and geophysical measurements of soil and sediment heterogeneity over a multi-month period. To calibrate our interpretations of the geophysical data we installed shallow groundwater monitoring wells and characterized soil cores (~1 m) at strategic locations for soil properties and microbial composition. Soil mineralogy was also determined by synchrotron-based X-ray diffraction. To our knowledge, this kind of integrated characterization has not been completed prior to the beginning of an ecosystem climate-change experiment, and it has had an impact on site understanding and experimental design.

Geophysical surveys by electrical resistivity tomography (ERT) and electromagnetic induction (EMI) revealed levels of heterogeneity within the study site that were not apparent either from surface observations or through traditional soil coring. We are testing whether the observed soil texture, and its pattern with depth, can be extrapolated to the site using ERT. The instrumented shallow piezometers have shown that water table fluctuations at the site are more dramatic than was expected. In the wet season, the water table rises as high as ~0.8 m below the ground surface in the vicinity of the study plots, well within the ~ 120 cm vertical region of interest (and heating) for this project.

These results have brought into focus important processes, such as redox variation, while the water table fluctuations will allow us to investigate the coupling between temperature and interannual moisture variations. The integrated picture informs the design of the heating treatments and the experimental layout, and will make the interpretation of future experimental results more robust. We will implement a regression design with multiple heating levels (+3 and +6 °C), and minimize intra-block variation and locate blocks across the landscape based on ERT and EMI results to explore the natural gradient in moisture, parent material, and vegetation. This will allow us to better elucidate the impacts of soil warming on ecosystem dynamics and threshold responses. In addition, by better incorporating the site hydrology in our understanding we will create a stronger connection between this project and other BER-funded efforts on water impacts and coastal exports.

Title: Microbial Exoenzyme Kinetic Traits Vary with Soil Depth but Have Similar Temperature Sensitivities Through the Soil Profile

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BER Program: TES

Project: Belowground Biogeochemistry SFA (lead: LBNL)

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

Project Abstract: The microbial mechanisms controlling soil organic matter (SOM) decomposition with warming are not well understood, particularly in subsoils, although they contain over 50% of global soil carbon. Deep soils have different physicochemical properties, nutrient inputs, and microbiomes, but it is not known if these lead to different SOM dynamics and temperature responses. In the LBNL Belowground Biogeochemistry SFA, 4.5 years of whole-profile soil warming at Blodgett Forest, CA, have led to higher microbial growth rates and modest depth-dependent changes in microbiome composition and metabolic potential. However, microbiomes in deeper soils have lower growth rates, carbon use efficiency, and potential to produce carbohydrate-active enzymes. We hypothesized that kinetics and temperature sensitivity of microbial exoenzymes, which mediate SOM depolymerization, vary with soil depth, reflecting adaptation to distinct substrate and temperature regimes. We determined the Michaelis-Menten (MM) kinetics of three ubiquitous enzymes involved in carbon (C), nitrogen (N) and phosphorus (P) acquisition at six soil depths to 90 cm, and their temperature sensitivity between 4-50°C based on Arrhenius and Macromolecular Rate Theory (MMRT) models. Maximal enzyme velocity (V_{max}) decreased strongly with depth for all enzymes, on a soil mass or microbial biomass basis, whereas their affinities increased, indicating adaptation to lower substrate availability. However, microbial biomass-specific catalytic efficiencies (CE) of C- and N-acquiring enzymes also decreased with depth, indicating that deep soil microbiomes encode enzymes with intrinsically lower turnover and/or produce less enzymes per cell, likely reflecting distinct life strategies. V_{max} and CE increased with warming, leading to higher SOM decomposition potential at all depths. This temperature sensitivity was similar through the soil profile based on Arrhenius/Q_{10} and MMRT models, similar to what has been observed for soil respiration. However, temperature sensitivity varied between enzyme types in a depth-dependent manner, implying changes in the

potential for depolymerization of different SOM compounds with warming down the profile. We are currently investigating the temporal and temperature responses of microbial trait distributions and expression as a function of depth, based on multi-omics approaches, and linking them to experimentally verified functional properties. Our results indicate that soil microbiomes have distinct functional traits and life strategies at depth, which may be fundamental determinants of biogeochemical cycling and responses to warming. In particular, enzyme kinetics and thermodynamics may represent inherent traits of soil microbiomes at depth, and prompt a more detailed, depth-resolved representation of enzyme-mediated processes in models of SOM dynamics.

The Watershed Function SFA: Mountainous System Hydrobiogeochemical Response to Disturbance across Genome to Watershed Scales

Susan Hubbard[1], Deb Agarwal[1], Bhavna Arora[1], Jillian Banfield[1,2], Nicholas Bouskill[1], Eoin Brodie[1], Rosemary Carroll[3], Dipankar Dwivedi[1], Ben Gilbert[1], Reed Maxwell[4], Michelle Newcomer[1], Peter Nico[1], Carl Steefel[1], Heidi Steltzer[5], Tetsu Tokunaga[1], Charu Varadharajan[1], Haruko Wainwright[1], Kenneth H. Williams[1] and the Watershed Function SFA Team

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BER Program: ESS
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Abstract: Uncertainty associated with predicting watershed hydrobiogeochemical behavior remains high as climate change, wildfire, land-use change, and other disturbances significantly reshape interactions within the world's watersheds. The Watershed Function SFA ("SFA") is reducing this uncertainty through advancing a predictive understanding of how **mountainous watersheds retain and release water, nutrients, carbon, and metals, particularly in response to snow dynamics and disturbances such as droughts, floods and wildfire.** The project is being undertaken at the mountainous headwater East River Watershed of the Upper Colorado River Basin. Streamflow originating from snowpack in this Basin provides the majority contribution to the Colorado River, which is critical for Western U.S communities, energy, agriculture, and industry.

The responses of mountainous systems to disturbance are particularly complex, involving multi-physics, multi-scale processes occurring from bedrock through canopy, across land-water interfaces, from genome-to-watershed scales and across extreme lateral gradients in elevation, vegetation and geology. To tractably confront this complexity, the SFA is developing new ways of conceptualizing, characterizing and predicting aggregated watershed system behavior. In particular, the SFA takes a system-of-systems approach, using remotely sensed and other information to identify key watershed subsystems or "functional zones". These zones are hypothesized to have unique properties (relative to neighboring parcels) that influence that zone's response to disturbance. To test the SFA functional zone concept, observations, experiments and modeling are performed within distinct, archetypal parcels to provide insights about how zones uniquely respond to snow dynamics. This information is in turn used to inform larger-scale predictions of aggregated, time-variable watershed concentration-discharge signature, using scale-adaptive watershed simulation (SAWaSC) and functional zone modeling capabilities. The SFA current phase focuses on developing a predictive understanding of aggregated water and nitrogen exports in response to snow dynamics.

The Watershed Function SFA has realized significant progress during this reporting period, leading to 54 papers that are published or in review. Select examples of progress this year include:

- Quantification of precipitation partitioning as a function of season and watershed characteristics and documentation that monsoons are not likely to compensate for decreased snowmelt in terms of streamflow generation;
- Deep quantification of the East River microbiome and how it varies with vegetation type, river meander and hillslope characteristics, and snowmelt dynamics;
- Quantification of the role and magnitude of bedrock weathering on watershed nitrogen exports and the first watershed-wide simulation of nitrogen cycling and exports;
- Developed and successfully tested a watershed zonation construct, finding that the extreme watershed heterogeneity could be accurately and tractably represented using just six zones;
- Acquired and archived a staggering diversity and volume of data from the East River site, which now includes >600 physical sensors, >100 million data points, and >100 data types.

Reconciling Evapotranspiration – Cross Method Synthesis, Uncertainty Quantification, and Path Forward

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BER Program: ESS
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Abstract: Accurate quantification of evapotranspiration (ET) is a common and fundamental challenge in predicting watershed hydrological behaviors. Large ET uncertainties stem from a multitude of sources depending on method-of-choice and scale. Two major factors are contributing to ET uncertainties and the difficulties in reconciling discrepancies among different methods, namely (a) unknown true ET values, and (b) differences in meteorological inputs and ET formulations. Understanding sources of uncertainty and developing gold-standard benchmarking platforms and datasets are key to accurately predicting ET rates and drivers at watershed scales and beyond.

We summarize recent progresses of the Watershed Function SFA on these challenges, highlighting (a) development of ET benchmarking platforms and datasets, and (b) reconciliation of various ET methods used at East River to identify sources of uncertainties. Combining these efforts will lead to significant improvements of ET quantification from local to watershed scales at the East River and beyond.

Specifically, gold-standard, best-in-practice methods were established at both the laboratory and field scales to for ET benchmarking. These include the lysimeter style SMARTSoils testbed at the Berkeley lab, and Eddy Covariance/Energy Balance systems, flux tent, water mass-balance, and sap-flow datasets in the field. The reconciliation efforts explored a multitude of ET methods, ranging from physics rich Penman Monteith model to petrophysics style models such as Priestley-Taylor, and across spatiotemporal scales from sub-minute to year-around meter scales at intensive sensing sites to multi-decadal studies across the East River watershed. We also included a wide range of methodologies ranging from stand-alone ET formulations to comprehensive modeling platforms, to isotopes.

While ET estimates vary significantly among different methods, there is consensus regarding transitions between water and energy limited systems across locations and years, and the need to understand the differing mechanistic drivers and responses for evaporation (E) and transpiration (T) across functional zones. Further, all methods point to the lack of true ET datasets for model

parameterization and benchmarking, and the inconsistency and insufficiency of meteorological and soil/plant measurements in resolution and scales, both of which calls for the consistent use of high-quality datasets across all methods. Continuing efforts will focus on the alignment of different methods on a common set of benchmarking locations, such as the pumphouse hillslope and Snodgrass intensive sites, and the collection and utilization of gold-standard datasets discussed above for model validation and improvements, which include the upcoming SAIL campaign that produces high quality meteorological data.

Carroll, R.W.H., Gochis, D., Williams, K.H., 2020. Efficiency of the summer monsoon in generating stream flow within a snow-dominated headwater basin of the Colorado River. Geophys. Res. Lett. 47, doi10.1029/2020GL090856

Chen, J., B. Dafflon, A. P. Tran, N. Falco, and S. S. Hubbard (submitted), A Deep-Learning Hybrid-Predictive-Modeling Approach for Estimating Evapotranspiration and Ecosystem Respiration, Hydrology and Earth System Sciences, DOI: 10.5194/hess-2020-322.

Ryken, A., Gochis, D., Maxwell, R. Unraveling groundwater contributions to evapotranspiration in a mountain headwaters: Using eddy covariance to constrain water and energy fluxes in the East River Catchment. Submitted to Hydrological processes. DOI: 10.22541/au.160974909.94645181/v1

Snowmelt Dynamics and its Contributions to Catchment Water Partitioning

Matthias Sprenger[1]*, Rosemary W.H. Carroll[2], Erica Woodburn[1], Baptiste Dafflon[1], P. James Dennedy-Frank[1], Kenneth H. Williams[1], Jeffery Deems[3], Reed Maxwell[4], Wendy Brown[5], Alexander Newman[5], Curtis Beutler[5], Markus Bill[4], Stijn Wielandt[1], Sebastian Uhlemann[1], Susan Hubbard[1]

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Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Abstract: We describe investigations combining observations and simulations of hydrometric (precipitation, discharge, snowpack) and stable isotope (^{2}H &^{18}O) data to infer the role of snowmelt in discharge generation in Colorado's East River Watershed. The first investigation assesses mechanisms of snowpack isotopic loading into the soil and the impact on recharge dynamics using PRMS coupled to a new snow isotope fractionation model (Carroll et al., in review). The latter was calibrated to observed spatiotemporal variability of snowpack volume and isotopes. We found that seasonal variability and elevation primarily control volume and isotopes of influx, and that snowpack isotopic fractionation via evaporation and melt account for only <5% of the influx variability. Our modelling indicates that recharge is highest in the upper subalpine. The simulated isotopes in this zone match groundwater observations, providing evidence that the upper subalpine is a preferential recharge zone in mountain systems.

In a second investigation, we infer rain vs. snow contributions to evapotranspiration and summer discharge using isotope mass balance approaches in seven East River subcatchments. The results confirm that snow dominates evapotranspiration and summer discharge (ca. 80%). About 50% of rainfall evapotranspired and <20% became summer discharge. Tree density best explains inter-catchment variability, as subcatchments with higher tree density have a larger share of evapotranspiration sourced by rain, more rain evapotranspiring, and less rain sustaining summer discharge. These findings agree with recent PRMS simulations showing monsoon rain cannot replenish water deficiency from lower snowpack (Carroll et al., 2020).

Particle tracking from an integrated hydrologic model (ParFlow-CLM-EcoSLIM) shows agreement with the isotope mass balance for ET fraction from snow across subcatchments. However, the two methods have differences in evapotranspiration sums, driving substantial mismatch in the fraction of snow evapotranspired. Future work will reconcile these differences by determining the effects on mass balance of groundwater storage changes and uncertainties in precipitation forcing.

To better assess the variability in snowpack thickness, snowmelt timing, and soil freeze-thaw intensity, we deployed a sensor network of a Distributed Temperature Profiling system developed at Berkeley Lab across 30 locations monitoring soil and snow temperature with unprecedented spatiotemporal resolution. The measurements indicate strong impacts of slope and aspect on the

snowpack dynamic, with South-West facing slopes without soil freezing and first bare-ground date up to one month earlier than the North-East facing slopes.

These approaches shed critical light on the timing and volume of snowmelt as a driver for heterogeneous hydrological responses in mountainous watersheds.

Carroll, R.W.H., Gochis, D., Williams, K.H., 2020. Efficiency of the summer monsoon in generating stream flow within a snow-dominated headwater basin of the Colorado River. Geophys. Res. Lett. 47, doi10.1029/2020GL090856

Carroll, R.W.H., Deems, J., Maxwell, R, Sprenger, M, Brown, W, Newman, A., Beutler, C, Bill, M, Hubbard, S, Williams, K.H., in review. Stable Water Isotope Loading Across Mountain Landscapes, Water Res. Res.

Leveraging Genomes for Quantitative Insights into Microbiome Influence on Watershed Function – a synthesis from the Watershed SFA at East River, CO

Patrick Sorensen[1*], Eoin Brodie[1,2], Jill Banfield[1,2], Nick Bouskill[1], Romy Chakraborty[1], Dipankar Dwivedi[1], Patricia Fox[1], Ben Gilbert[1], Ulas Karaoz[1], Junhyeong Kim[1], Adi Lavy[2], Paula Matheus Carnevali[2], Hannah Naughton[1], Michelle Newcomer[1], D. Brian Rogers[3], Alex Thomas[2], Shi Wang[1], Xiaoqin Wu[1] and the Watershed Function SFA team

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BER Program: ESS
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Abstract: Scaling microbiome processes to watershed or basin scales is a challenge due to the fine scale at which microbes interact with their environment. An open research question in watershed science is to what extent microbiome properties affect aggregated watershed functions? The Watershed Function SFA, aims to develop a predictive understanding of aggregated watershed responses to perturbations. We hypothesize that the spatial distribution of microbial functional traits can improve predictions of aggregated watershed function in space and time. We are testing this hypothesis through 1) strategic field sampling of metagenomes in key watershed locations during critical periods of the hydrologic cycle (e.g., snowmelt or baseflow), 2) targeted lab experiments to discover the diagnostic microbial metabolic pathways responsible for nutrient retention versus loss, 3) use of metabolomics and genome-inferred traits to parameterize reactive transport models. To facilitate this watershed scale synthesis, we are constructing an interoperable and reusable resource for all microbial multi-omic, microbial trait, and soil biogeochemical data collected from East River.

Across seven synergistic campaigns microbial processes have been interrogated along a continuum from bedrock to canopy, focused on key watershed domains including upland hillslopes, multiple meanders along the river corridor, and at mineral weathering interfaces in the subsurface or the rhizosphere. Topographic position in the landscape, vegetation type, and snowpack properties all shape microbiome features, although we have observed remarkable consistency in genome and functional trait frequency in specific watershed domains. An intensive field campaign was carried out, where 400 samples were obtained from 13 locations across four catchments in the upper East River watershed varying in elevation, hydrological and geological properties, and dominant vegetation types. This was concurrent with an NSF NEON Airborne Observatory Platform imaging flight (hyperspectral and LiDAR) over the study area. In partnership with the JGI, we have obtained 724 metagenome samples, completed assemblies from 511 and binning of 371, together comprising at least 91K microbial species. We are currently synthesizing these observations, using genome-inferred traits to define microbial functional guilds and their watershed scale distributions. Integration of airborne remote sensing surveys (geomorphology, snowpack and vegetation distributions), plus advanced geophysical sensing allows quantification of co-variance between microbiomes, soil biogeochemistry and surface observable properties. This information allows us to parameterize genome-informed reaction networks and their microbial

kinetics, and using machine learning approaches, to derive suites of surface observables properties that are predictive of microbial functional trait and genome distributions across the watershed.

Lavy, A., McGrath, D. G., Matheus Carnevali, P. B., Wan, J., Dong, W., Tokunaga, T. K., ... & Banfield, J. F. (2019). Microbial communities across a hillslope-riparian transect shaped by proximity to the stream, groundwater table, and weathered bedrock. Ecology and evolution, 9(12), 6869-6900.

Carnevali, P.B.M., Lavy, A., Thomas, A.D., Crits-Christoph, A., Diamond, S., Méheust, R., Olm, M.R., Sharrar, A., Lei, S., Dong, W. and Falco, N., 2021. Meanders as a scaling motif for understanding of floodplain soil microbiome and biogeochemical potential at the watershed scale. Microbiome, 9(1), pp.1-23.

Sorensen, P. O., Beller, H. R., Bill, M., Bouskill, N. J., Hubbard, S. S., Karaoz, U., ... & Brodie, E. L. (2020). The snowmelt niche differentiates three microbial life strategies that influence soil nitrogen availability during and after winter. Frontiers in Microbiology, 11, 871.

Chadwick, K. D., Brodrick, P. G., Grant, K., Goulden, T., Henderson, A., Falco, N., ... & Maher, K. (2020). Integrating airborne remote sensing and field campaigns for ecology and Earth system science. Methods in Ecology and Evolution, 11(11), 1492-1508.

Bedrock–Watershed Connections and Conundrums

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BER Program: ESS
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Abstract: Bedrock stores and releases water, nutrients and chemical energy on a large range of timescales. Sedimentary rock, for example, can preserve for millions of years organic molecules generated by ancient biological carbon and nitrogen fixation, and reactive minerals precipitated through biogeochemical processes. Uplift and exposure of bedrock initiates chemical and biological weathering that mobilizes these elements into groundwater and back into terrestrial biogeochemical cycles. On the seasonal-to-decadal timescale, fractured and porous bedrock can transiently store water, organic and inorganic carbon, and other redox-active elements as precipitation patterns and groundwater transport vary. The ecological impacts of bedrock in mountainous watersheds, which are often water- and nutrient-limited, and which experience relatively fast rates of weathering, can be particularly important but remain poorly quantified.

The Watershed Function SFA, located in the snow-dominated mountainous headwaters of the East River, CO, and surrounding catchments, is revealing the roles for bedrock as a reservoir of water and elements. Groundwater and subsurface gas measurements have shown that the weathering of organic-rich marine shale can be a significant source of biologically available nitrogen (*Wan et al.,* 2021). High-resolution imaging of the records of rock weathering have established the geochemical reaction networks controlling the release of elements to groundwater (*Lavy et al.,* 2019). Distributed metagenomic studies have connected rock-derived elements to microbial metabolism and found that proximity underlying Mancos shale apparently controls species distribution (*Carrero Romero et al.*, in prep). Watershed-scale geophysical and remote sensing are establishing how bedrock composition (e.g., types, hydrothermal alteration), topography and subsurface structure influence vegetation distribution and susceptibility to drought. Soil-to-bedrock vegetation harvesting discovered deep roots of perennial shrubs to penetrate to regions of weathering bedrock, suggesting a strategy for acquisition of water or nutrients. High-frequency stream water measurements uncovered distinctive trace-element patterns likely caused by motions on the faults or fractures connecting from subsurface rocks to the watershed.

These findings demonstrate multiple ways in which bedrock and surficial processes are connected, but questions and challenges remain. In particular, the ecohydrogeological factors that determine the biogeochemical retention, cycling or export of bedrock derived elements remain to be

established and quantitatively scaled across this geomorphologically diverse landscape. Although measurement and modeling of the trends in chemical composition of the East River and its tributaries can distinguish impacts of watershed processes (*Arora et al.,* 2020), understanding the temporal and climate feedbacks between rock, plant and microbial processes that control water and element retention or loss remains an ongoing objective addressed through new studies in and around this catchment.

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Towards a Conceptual Framework of Watershed Nitrogen Retention and Loss across Scales

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Abstract: Patterns of watershed nitrogen (N) retention and loss are shaped by how watershed mechanistic processes retain, biogeochemically transform, and lose incoming atmospheric and geogenic sources of N. Recent studies in snowmelt-dominated catchments have documented changes in nitrogen (N) retention over time, such as declines in watershed exports of N (*Newcomer et al.,* 2021), though a comprehensive framework accounting for process-based interactions operating at different spatial and temporal scales is still missing. Synthesizing experimental and modeling N-studies in the East River, we assess application of the novel Watershed Index for Retention and Loss (WIRL) concept as it relates to N.

Our synthesis aggregates local-to-basin scales using 1500 datapoints of concentration-discharge (C-Q) signals, subsurface/surface/soil/plant sampling across different compartments and ecoregions, paired-catchment analysis, and subsurface and surface modeling down the river corridor. The WIRL concept suggests that functional information about the landscape (retention and loss) can be found within signals that aggregate those mechanisms. C-Q signals in the river corridor are one such example of a signal that aggregates information from the landscape. An examination of differential C-Q signals at three main East River sites, each near floodplain riparian zones, suggest the meandering downstream section is marked by gains in both groundwater and NO_3^- concentrations as opposed to the dilution and the declining trends observed in the high-relief, steep terrain upstream reach (*Arora et al.,* 2020). Modeling work at the local and watershed scales help to narrow the range of mechanisms controlling the observed C-Q trends. At the local scale, modeling of floodplain riparian hollows suggest they functionally act as inhibitors to upland hillslope NO_3^- reaching the stream (35-55% removed) (*Rogers et al.,* 2021). At the watershed scale, we developed the High-Altitude Nitrogen Suite of Models (HAN-SoMo), a watershed-scale ensemble of process-based models of the East River Watershed (*Maavara et al.,* 2021). While geogenic sources account for approximately 12% of the annual dissolved N sources to the watershed, on an annual scale, instream dissolved N elimination, plant turnover (including cattle grazing) and atmospheric deposition are the most important controls on N cycling. These studies reveal that retention of N in subsystems of the watershed is highly heterogeneous and a potential function of presence or absence of floodplains, plant dynamics, and highlights the importance of

transformations once N reaches the stream. At the watershed and basin scale we validate the first application of the WIRL concept at an unprecedented scale across the CONUS that links instream nitrogen signals to upstream mechanistic landscape processes (*Newcomer et al.,* 2021).

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Advanced bedrock characterization of a mountainous watershed using geological and geophysical data, and machine learning

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Abstract: Bedrock properties are critical for understanding and predicting the hydrological response of watersheds to climate disturbances. Estimating these properties on a watershed-scale is inherently difficult, particularly for fractured-bedrock dominated domains. Our analysis provides the first study to test the co-variability of above and below ground features on a watershed-scale, based on extensive airborne electromagnetic (AEM) data, surface and borehole geophysical data, and high-resolution remote sensing data. We use machine learning approaches to quantify the relationships between bedrock geophysical/hydrological properties and geomorphological/vegetation indices at the East River Watershed, CO, and show that these relationships can be used to estimate the first order variability of bedrock properties throughout the watershed. By assessing the stationarity of these relationships, we show that regions of smaller variability in the input parameters, i.e. slope, aspect, elevation, and vegetation cover, provide more accurate estimates of bedrock properties, highlighting the limitation of commonly applied geomorphological models that rely solely on above-/below-ground co-variability.

Through this analysis we identified previously unmapped fracture zones. To identify the origin of one such fracture zone, we developed a Popper-Bayes hypothesis testing method that incorporates machine learning elements. Based on this approach, we falsified several geological models, and concluded that the most likely origin of this fracture zone, which is crossing one of the Watershed intensive sites, is either a normal or high-angle reverse fault, or a potential sackung feature. This result implies that auxiliary features associated with the fracture zone, such as offset geological layers, may also be present in the watershed.

Combining these detailed studies of bedrock properties with state-of-the-art geological modelling approaches, we have developed a 3D geological model of the entire East River Watershed and beyond. This model, integrating various bedrock characterization approaches, is building the basis for novel flow and transport modelling tasks and targeted subsurface property investigations. These studies highlight that a multi-scale characterization of a watershed from plot to regional scale, as we performed, is required to enable detailed modelling of subsurface flow and transport to assess the impact of disturbances onto such hydrological systems.

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Watershed zonation approach for tractably quantifying above-and-belowground watershed heterogeneity and functions

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Abstract: Predictive understanding of watershed functions is often hindered by the heterogeneous and multiscale fabric of watersheds. In this study, we have developed a watershed zonation approach for characterizing watershed organization and functions in a tractable manner by integrating multiple spatial data and model output layers. Recognizing the coupled ecohydrogeological-biogeochemical interactions that occur across bedrock through canopy compartments of a watershed, we hypothesize that (1) suites of above/belowground properties co-varying with each other, (2) machine learning methods can be used to identify watershed zones having unique distributions of bedrock-through-canopy properties relative to neighboring parcels, and (3) property suites associated with the identified zones can be used to understand zone-based functions, such as response to early snowmelt or drought, evapotranspiration, and associated solute exports to the river. This zonation approach essentially reduces the complexity or multidimensionality of watershed heterogeneity into a set of zones.

We have explored multiple zonation constructs to capture multiscale natures of heterogeneity as well as various watershed patterns and functions – based on both observations and modeling results – at the East River Watershed near Crested Butte, CO. We first developed unsupervised clustering methods that synthesizes airborne remote sensing data (LiDAR, hyperspectral, and electromagnetic surveys) and bedrock-to-canopy co-variability. Using independently collected data, it is shown that the identified zones capture the heterogeneity of key watershed functions at the watershed scale, including foresummer drought sensitivity and river nitrogen exports. Second, we have applied unsupervised clustering to the input and output data layers of a watershed-scale integrated hydrological model, which found the co-variability of elevation and topographic metrics and key hydrological functions such as water table dynamics and evapotranspiration. In addition, at the hillslope scale, we have developed a zonation approach that captures plant dynamics time-series and soil moisture associated with microtopography. These results combined have contributed significantly to selecting hillslope experiment locations as well as optimizing a large-scale monitoring network of snow, precipitation, and soil moisture.

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Multiscale Analysis of Watershed Function with High Resolution Process-Based Models

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Abstract: We are using high-resolution process-based modeling to quantify aggregated water and biogeochemical cycling at the watershed scale. This modeling is carried out at multiple scales, beginning with individual soil pits and boreholes, extending to 2D hillslope and floodplain transects, 3D hillslope, and 3D sub-catchment scale, and combines both high-resolution surface-subsurface water modeling with reactive transport. Our ultimate objective is to quantify solute and nutrient export (especially nitrogen) to the stream network in the East River watershed, considering flow, bedrock weathering, and shallow soil and vegetation processes, all within the context of transient climate forcing and other disturbances.

This research component includes:

- *Zone-based transect modeling:* Functional zones have been identified that depend in part on the distinctive characteristics of the hillslopes. For each functional zone, we are creating a hillslope scale model (typically in 2D) to examine hillslope and floodplain connectivity that impacts river chemistry and comparing its response to early snowmelt. The analysis is also being extended to consider deep time weathering of bedrock to determine how this influences present day and future chemical export to the stream network.
- *Reduced dimension 1D modeling of flowtubes to represent hillslope fluxes:* With the development of a new computationally efficient approach to modeling transient flow and reactive transport in flowtubes, we are quantifying the aggregated hillslope fluxes to the stream network.
- *3D HPC modeling of surface+subsurface flow and biogeochemistry:* Using the software platform Amanzi-ATS, we are developing models for flow and biogeochemistry at the sub-catchment scale, initially focusing on the Copper Creek and the Lower Triangle. These computationally-intensive simulations provide direct predictions of C-Q responses in the East River system, while capturing the spatially-distributed processes that underpin these responses using multi-resolution meshes. They also provide synthetic data for machine-learning based reduced order models.
- *SAWASC: Functional Zone-based reduced-order modeling to predict Aggregated Watershed discharge and nitrogen export:* Building on insights from the HPC modeling task, a reduced-order SAWaSC (Scale Adaptive Watershed Simulation Capability) modeling approach is being developed to predict aggregated watershed discharge and nitrogen as a function of snow dynamics. The approach is based on a residence time analysis within stretches of the river system, with lateral bedrock and hyporheic exchange taken from *machine learning-based training* on the high resolution distributed HPC sub-catchment simulations of biogeochemical

cycling and fluxes. The zonation will be used to provide time-dependent lateral fluxes of water and biogeochemical species to the river system, i.e., C-Q relationships.

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Title: **The LLNL Biogeochemistry at Interfaces SFA**

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Project: LLNL DOE SFA: Biogeochemistry at Interfaces

Project Website: https://doesbr.org/research/sfa/sfa_llnl.shtml

Project Abstract: The focus of the BioGeoChemistry at Interfaces SFA is to identify and quantify the biogeochemical processes and the underlying mechanisms that control actinide and metal ion mobility to reliably predict their cycling and migration in the environment. The research approach includes: (1) Field studies that capture behavior on the timescale of decades and (2) Fundamental laboratory studies that isolate specific biogeochemical processes observed in the field. These efforts are underpinned by the unique capabilities and staff expertise at Lawrence Livermore National Laboratory, allowing the *BioGeoChemistry at Interfaces SFA* to advance our understanding of actinide and metal ion behavior in the environment, and serve as an international resource for environmental science and radiochemistry research.

Despite the challenges of the past year, our team has maintained its scientific productivity (10 manuscripts published/submitted), established a new ephemeral stream Test Bed at the Nevada National Security Site, hired two new postdocs (Naomi Wasserman and Teresa Baumer), and initiated a new focus area in machine learning in geochemistry. Exciting scientific results of the past year include 1) discovering how bacterial surfaces can facilitate the precipitation of U-phosphate minerals by providing a local environment that is supersaturated with respect to U-phosphate minerals (Morrison et al., 2021), 2) identifying how reducing conditions can lead to Fe and Pu mobilization in estuaries, 3) identifying the enhanced Fenton-type oxidation potential of surface water and shallow sediments in the presence of organic matter (Pan et al., 2021), and 4) identifying how subsurface planktonic microbial communities reflect regional-scale groundwater hydraulic connectivity and groundwater flow patterns (Merino et al., submitted).

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Title: **BioGeoChemical Cycling at a Monomictic Stratified Pond, Savannah River Site, SC**

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Project: LLNL DOE SFA: Biogeochemistry at Interfaces

Project Website: https://doesbr.org/research/sfa/sfa_llnl.shtml

Project Abstract: Pond B at Savannah River Site (SRS) is an ideal location for examining the biogeochemical cycling of Fe, Pu, organic matter, and other metals in a monomictic stratified pond. This pond received reactor cooling water from 1961–1964 containing trace levels of $^{238,239,240}Pu$, ^{137}Cs, ^{90}Sr, ^{241}Am, and ^{244}Cm. Since then, Pond B has remained relatively isolated except for a few studies conducted in the late 1980s, which demonstrated Pu cycling with seasonal anoxia. However, the mechanism(s) causing Pu mobilization have not been identified.

During summer stratification, Pu, Fe and ^{137}Cs aqueous concentrations increase with depth, consistent with historical observations and likely linked to reductive dissolution of Fe-(oxy)hydroxides and mobilization of organic matter. These trends are consistent with 1983 measurements of $^{239,240}Pu$ activity in Pond B, although Pu concentrations have since decreased 2- to 3-fold in the water column and slightly in the soil profiles. Pu isotopic ratios fall between accepted values for Northern Hemisphere fallout and previously recorded ratios at SRS. This range most likely reflects the mixing between atmospheric sources of Pu and historical releases into Pond B. Comparisons of the concentration profiles within soil cores help explain metal cycling in the water column. Total ^{239}Pu and ^{237}Cs from the inlet, the bank and outlet of the pond, show that Pu and Cs accumulation is largely restricted to the upper 5 cm of sediment and appears highly correlated with organic matter.

We found that the Pond B water microbial community varies with depth rather than location during stratification and can be categorized by the three distinct stratification layers. However, during spring turnover, the microbiome is homogenized throughout Pond B, reflecting the uniform geochemistry (e.g., oxygen concentrations, temperature, metals). Further analysis of the microbial community is ongoing, including identifying co-occurring microbes and ontological predictions of metabolisms and functions. Future analysis will also include the development of a database of iron oxidizers and reducers for predicting microbial iron redox functions using 16S rRNA amplicon sequencing data.

Title: **LLNL SFA Test Beds at the Ravenglass Estuary (UK), Hanford Site Vadose Zone, and Nevada National Security Site Ephemeral Stream**

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Project Abstract: The BioGeoChemistry at Interfaces SFA includes four test beds and one engineered field site that have been chosen based on their known contamination history, their range of contaminant loading, their location within watersheds, and the specific processes that are believed to control actinide transport. These test beds allow us to test our conceptual and mechanistic understanding of actinide migration using long-term field-specific contaminant migration information.

Ravenglass site (England) – Testbed to examine cycling in redox stratified sediments. The Ravenglass salt marsh is within the Sellafield site on the north west coast of England. Sellafield was originally established in 1947 to support the UK nuclear weapons program and effluents from this site are, by far, the largest source of Pu discharged in all of western Europe (276 kg Pu). The Ravenglass saltmarsh is a highly dynamic system located 10 km south of the Sellafield site and is a low energy, intertidal region that accumulates Sellafield-derived contamination. To determine the factors affecting the mobility of Pu in these redox stratified sediments, we conducted a series of desorption experiments under both oxic and anoxic conditions over a nine-month period. The results of this work suggest that Pu desorption (and mobilization) increases under anoxic conditions in estuary sediments. This is leading to a paradigm shift in our understanding of Pu redox chemistry and its impact on radionuclide migration.

Hanford site (Washington, US) – Testbed to examine legacy waste impacted conditions. The unlined Z-9 trench at the Hanford Reservation (200 Area) received large volumes (~$4x10^6$ liters) of Pu processing waste consisting of high salt (~ 5M NO_3, ~ 0.6M Al), acidic (pH ~ 2.5) solutions, which also contained the organic solvents: CCl_4, TBP, DBP, and lard oil. A small fraction of Pu migrated deep into the subsurface vadose zone to depths of 37 m. Binary batch experiments containing aqueous phase and organic phases demonstrated Pu was sequestered by the organic phase at pH 2 and 3 and partitioning decreased with increasing pH. Thus, Pu may be mobilized into the aqueous phase during infiltration of low ionic strength waters.

Nevada National Security Site (Nevada, US) – Testbed to examine wet-dry cycling using ephemeral stream beds. Ephemeral stream beds at Rainer Mesa, Nevada (site of nine underground nuclear tests) is used to evaluate the influence of stream bed wet-dry cycling on actinide migration. Continuous discharge from a perched aquifer drains into a series of unlined containment ponds located in an ephemeral stream bed. While radionuclide concentrations in the discharge remain below permissible limits, distribution of contaminants in the pond sediments and shallow groundwater underlying the ponds are unknown. In collaboration with Mission Support and Test Services, LLC, we conducted the first sampling trip to the E-Tunnel pond system in April 2021. Thirteen sediment cores (6" deep) were collected to examine actinide and trace metal distributions. Another sampling campaign is planned during wetter conditions to capture contaminant distribution in pond sediments and porewater in a fully saturated state.

Next-Generation Ecosystems Experiment (NGEE Arctic): Progress and Plans

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The Next-Generation Ecosystem Experiments (NGEE Arctic) project seeks to improve the representation of tundra ecosystems in Earth System Models (ESMs) through a coordinated series of model-inspired investigations conducted in landscapes near Utqiaġvik (formerly Barrow) and Nome, Alaska. In Phase 1 (2012 to 2014), we tested and applied a multiscale measurement and modeling framework in a coastal tundra ecosystem on the North Slope of Alaska. In Phase 2 (2015 to 2019), three additional field sites were established on the Seward Peninsula in western Alaska. Integrated field, laboratory, and modeling tasks allowed our team to focus on understanding (1) the effect of landscape structure on the storage and flux of C, water, and nutrients, (2) geochemical mechanisms responsible for CO_2 and CH_4 fluxes across a range of permafrost conditions, (3) variation in plant functional traits across space and time, and in response to changing environmental conditions and resulting consequences for ecosystem processes, (4) controls on shrub distribution and associated biogeochemical and biophysical climate feedbacks, and (5) changes in snow processes and surface and groundwater hydrology expected with warming in the 21st century. A major outcome of our Phase 1 and 2 research was an integrated set of in situ and remotely sensed observations that quantify the covariation of hydro-thermal, ecosystem, vegetation dynamics, and biogeochemical function. Now in Phase 3 (2020 to 2022) we build upon our research at sites on the North Slope and in western Alaska, while also adding a cross-cutting component on disturbance. Field campaigns, modeling, and data synthesis are used to target improvements in simulating disturbance-related processes (e.g., wildfire and abrupt permafrost thaw) and connections to dynamic vegetation (e.g., shrubs) that are missing from or poorly represented in ESMs. Our vision strengthens and extends the connection between process studies in tundra ecosystems and high-resolution landscape modeling and scaling strategies developed in Phases 1 and 2. Safety, national and international collaboration, and a commitment to diversity and inclusion continue to be key underpinnings of our research approach and team philosophy in the Arctic.

Integrating Arctic Vegetation Types into the E3SM Land Model Using Above- And Below-Ground Field Observations

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Accurate simulations of high latitude ecosystems are critical for confident Earth system model projections of carbon cycle feedbacks to global climate change. Land surface models, including the E3SM Land Model (ELM), simulate vegetation growth and ecosystem responses to changing climate and atmospheric CO_2 concentrations by grouping heterogeneous vegetation into plant functional types (PFTs), which can be defined at varying levels of detail. Many ecosystem models represent high-latitude vegetation using only two PFTs representing shrubs and grasses, thereby missing the diversity of vegetation growth patterns in the Arctic. This study used field observations of above- and belowground vegetation biomass and traits across a gradient of plant communities on the Seward Peninsula in northwest Alaska to incorporate nine Arctic-specific PFTs into ELM. The newly developed PFTs included: 1) mosses and lichens, 2) deciduous and evergreen shrubs of various height classes, including an alder shrub PFT, 3) graminoids, and 4) forbs. Improvements relative to the original model configuration included greater belowground biomass allocation, persistent fine roots and rhizomes of nonwoody plants, and better representation of variability in total plant biomass across sites with varying plant communities and depths to bedrock. Simulations through 2100 showed alder-dominated plant communities gaining more biomass and lichen-dominated communities gaining less biomass compared to original model PFTs. Our results highlight how representing the diversity of arctic vegetation and confronting models with measurements from varied plant communities improves the representation of arctic vegetation in terrestrial ecosystem models.

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Alaskan Carbon-Climate Feedbacks to Press and Pulse Disturbances

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Land carbon-climate feedbacks represent a significant uncertainty in predicting atmospheric carbon concentrations under a changing climate. This study applies a well-tested mechanistic land model to examine how different disturbances can lead to non-linear feedbacks to the carbon cycle in high-latitude ecosystems. We first examine the Alaskan ecosystem response to warming. Short-term field experiments project warming to stimulate soil organic matter decomposition, and promote a positive feedback to climate change. We simulate both decade-long, acute warming experiments, and multi-decadal, chronic warming consistent with a changing climate. Herein, we show that the tightly coupled, nonlinear nature of high-latitude ecosystems implies that short-term (<10 year) warming experiments produce emergent ecosystem carbon stock temperature sensitivities inconsistent with emergent multi-decadal responses. In particular, short-term warming manipulations do not capture the non-linear, long-term dynamics of vegetation, and thereby soil organic matter, that occur in response to thermal, hydrological, and nutrient transformations belowground under chronic changes in climate. We expand on this work by examining the impact of pulsed disturbances (i.e., wildfire) on Arctic carbon cycling occurring against a backdrop of warming, altered precipitation, and elevated CO_2. Alongside rapid periods of warming, tundra ecosystems have experienced an increased frequency of fire in recent decades, and this trend is predicted to continue throughout the 21st Century. The post-fire recovery of these ecosystems is underpinned by complex interactions among microbial functional groups that drive carbon and nutrient cycling following a fire. We applied a series of climate change simulations with and without fire to ascertain how tundra ecosystems recover post-disturbance. These model scenarios include two temporally distinct ecosystems: (1) an early century, graminoid dominated ecosystem consistent with current conditions and (2) a late century ecosystem with elevated shrub abundance. We use the model to demonstrate an acceleration of the nitrogen cycle post-fire that is driven by changes in niche space and microbial competitive dynamics. Post-fire recovery is slower at the beginning of the 21st century compared to the onset of fire later in the century, due to warming-induced elevated nutrient availability. We conclude that consideration of distinct microbial metabolisms related to carbon and nutrient cycling are important when considering ecosystem recovery rates following disturbance.

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High-Resolution Modeling of Permafrost Dynamics in Seward Peninsula, Alaska

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We apply a transient temperature dynamic model to investigate the spatiotemporal evolution of permafrost conditions on the Seward Peninsula, Alaska—a region currently characterized by continuous permafrost in its northern part and discontinuous permafrost in the south. We calibrate model parameters using a data assimilation technique exploiting historical ground temperature measurements collected across the study area. The model is then evaluated with a separate control set of the ground temperature data. Calibrated model parameters are distributed across the domain according to ecosystem types. The forcing applied to our model consists of historic monthly temperature and precipitation data and climate projections based on the Representative Concentration Pathway (RCP) 4.5 and 8.5 scenarios. Simulated near-surface permafrost extent for the 2000–2010 decade agrees well with existing permafrost maps and previous Alaska-wide modeling studies. Future projections suggest a significant increase (3.0°C under RCP 4.5 and 4.4°C under RCP 8.5 at the 2 m depth) in mean decadal ground temperature on average for the peninsula for the 2090–2100 decade when compared to the period of 2000–2010. Widespread degradation of the near-surface permafrost is projected to reduce its extent at the end of the 21st century to only 43% of the peninsula's area under RCP 4.5 and 8% under RCP 8.5.

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Thawing Permafrost May Cause Headwater Streams to Cool

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The presence, continuity, and depth of permafrost significantly affects the flow of water through Arctic landscapes and thus potentially impacts stream discharge and thermal regimes. Analyses [1] of July water temperatures from 11 headwater streams in Alaska revealed higher temperatures in catchments with more near-surface permafrost. We used [1] the fully coupled cryohydrology model ATS [2,3] to investigate if deeper flow paths caused by thawing permafrost could create the same trend in the temperatures of groundwater discharging from hillslopes to streams. ATS simulates surface energy and water balances, snow thermal processes, and integrated surface/subsurface water flow and energy transport. We configured ATS to represent two-dimensional hillslopes with varying permafrost extent and found that hillslopes with continuous permafrost have shallower flow paths and twice as high rates of evapotranspiration, compared to hillslopes with no permafrost. For our simulated cases, the horizontal water flux moving through the top organic soil layers was more than ten times greater in continuous permafrost compared to permafrost-free cases. The deeper flow paths in the permafrost-free cases buffer seasonal temperature extremes. As a result, the summer groundwater temperatures discharging to streams are highest with continuous permafrost, consistent with the observations. Our results suggest that permafrost thaw will alter groundwater flow paths, reduce evapotranspiration, and result in more and cooler groundwater discharge to streams in the summer. The cooler groundwater discharging to stream will at least partially compensate for greater stream heating by warmer air, which has important implications for temperature-sensitive fish species. The previously unidentified negative feedback process will be strongest for headwater streams that are dominated by groundwater inflows. Additional work is required, however, to quantify the relative importance of direct stream heating and cooler groundwater inflows and how the relative importance changes with stream order.

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Future Increases in Arctic Lightning and Fire Risk for Permafrost Carbon

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Lightning is expected to increase at high latitudes under expected 21st century climate change. Using satellite-observed lightning flash rate and a climate reanalysis product, we found that summer lightning over northern circumpolar regions currently exhibits a strong positive relationship with the product of convective available potential energy (CAPE) and precipitation. Using Climate Model Intercomparison Project Phase 5 (CMIP5) climate projections for the RCP8.5 scenario, we identified increases in CAPE (86 ± 22%) and precipitation (17 ± 2%) in areas underlain by permafrost by the end of the century; these changes will cause summer lightning to increase by 112 ± 38%. Future flash rates at the northern treeline are comparable to current levels 480 km to the south in boreal forests. We are extending this work by simulating these increases in flash rates and thereby fires across Alaska in the *ecosys* model to explore effects on carbon cycling. Our preliminary results indicate that warmer climate, and elevated atmospheric CO_2 resulted in greater gains in plant biomass. However, increased soil organic carbon (SOC) losses resulted from (1) wildfire combustion and (2) rapid SOC decomposition primed by vegetation changes that led to increased deciduous litter. These SOC carbon losses offset the modeled plant carbon gains, leading to Alaska becoming a net carbon source to the atmosphere after year 2100.

Reference

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Arctic Soil Patterns Analogous to Fluid Instabilities

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Slow-moving arctic soils form patterns resembling those found in common fluids, such as paint and cake icing drips. Though these features impact hillslope stability, carbon storage and release, and landscape response to climate change, no mechanistic explanation exists for their formation. Inspired by fluid instabilities, we develop a new conceptual model for soil patterns and use mathematical analysis to predict their wavelength. We propose that soil patterns arise due to competition between gravity and cohesion, or the "stickiness" of soil grains. We compare our theoretical predictions with a large new data set of soil features from Norway, finding that soil patterns are controlled by both fluid-like properties as well as climate. We also present a comprehensive compilation of solifluction velocity profiles found in the literature and calculate the effective viscosity of soil for field sites across the globe. This informs our understanding of soil rheology, and therefore how soil may respond to changes in climate and hydrologic forcing. Our work proposes a new framework for thinking about Arctic soil stability. Findings may be used as a launching point to improve modeling efforts that predict cohesion-controlled topographic roughness and its role in modulating hillslope hydrology, slope stability, and carbon storage and release. More broadly, results provide the first physical explanation for a common pattern on both Earth and Mars, with implications for our understanding of landscapes and complex materials composed of both granular and fluid components.

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Geophysical Monitoring Shows that Spatial Heterogeneity in Thermohydrological Dynamics Reshapes Transitional Permafrost Systems

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Climate change is causing rapid changes of Arctic ecosystems. Yet, data needed to unravel complex subsurface processes are very rare. Using geophysical and in situ sensing at the NGEE-Arctic Teller Watershed near Nome, AK, we closed an observational gap associated with thermo-hydrological dynamics in discontinuous permafrost systems. Monitoring for more than 2 years, our data highlight the impact of vegetation, topography and snow thickness distribution on subsurface thermo-hydrological properties and processes. Large snow accumulation near tall shrubs insulates the ground and allows for rapid and downward heat flow during snowmelt and rain events. Thinner snowpack above the graminoid leads to surficial freezing and prevents water from infiltrating into the subsurface. Analyzing short-term disturbances such as snowmelt or heavy rainfall, we found that lateral flow could be a driving factor in talik formation. Linking our field data with laboratory derived property-relationships, we show that deep permafrost temperatures increased by about 0.2°C over 2 years. By highlighting the link between above and below ground properties and processes in the Arctic, our results will be useful for improving predictions of Arctic feedback to climate change. They also show that Arctic warm permafrost systems are changing rapidly. For instance, our data suggests that permafrost at our study site could disappear within the next decade. This process could be accelerated by changes in subsurface permeability, snowpack distribution and rainfall patterns. Building upon this work and in order to study dynamics across a range of vegetation type and landscape positions, we installed an additional monitoring transect at a nearby location characterized by colder subsurface temperature. The data from the two sites allow us to compare thermal-hydrological dynamics across elevation, slope, and vegetation types, and is supported by a network of depth-resolved temperature measurements that were deployed through the watershed. Using this data, we will quantify links between surface features and subsurface conditions and processes, which will allow us to upscale our site-scale observations to a regional scale, and will further improve our observational understanding of the impact of climate warming on the thermo-hydrological characteristics of Arctic environments.

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Topographical Controls on Hillslope-Scale Hydrology Drive Shrub Distributions on the Seward Peninsula, Alaska

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Observations indicate shrubs are expanding across the Arctic tundra, mainly on hillslopes and primarily in response to climate warming. However, the impact topography exerts on hydrology, nutrient dynamics, and plant growth can make untangling the mechanisms behind shrub expansion difficult. We examined the role topography plays in determining shrub expansion by applying a coupled two-dimensional version of a mechanistic ecosystem model (ecosys) in a tundra hillslope site in the Seward Peninsula, Alaska. Modeled biomass of the dominant plant functional types agreed very well with field measurements ($R^2 = 0.89$) and accurately represented shrub expansion over the past 30 years inferred from satellite observations. In the well-drained crest position, canopy water potential and plant nitrogen (N) uptake was modeled to be low from plant and microbial water stress. Intermediate soil water content in the mid-slope position enhanced mineralization and plant N uptake, increasing shrub biomass. The deciduous shrub growth in the mid-slope position was further enhanced by symbiotic N_2 fixation primed by increased root carbon allocation. The gentle slope in the poorly drained lower-slope position resulted in saturated soil conditions that reduced soil O_2 concentrations, leading to lower root O_2 uptake and lower nutrient uptake and plant biomass. A simulation that removed topographical interconnectivity between grid cells resulted in (1) a 28% underestimate of mean shrub biomass and (2) over or underestimated shrub productivity at the various hillslope positions. Our results indicate that land models need to account for hillslope-scale coupled surface and subsurface hydrology to accurately predict current plant distributions and future trajectories in Arctic ecosystems.

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Iron and Iron-Bound Phosphate Accumulate in Surface Soils of Ice-Wedge Polygons in Arctic Tundra

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The arctic tundra stores large quantities of soil organic carbon (C) that can be converted to greenhouse gases and released to the atmosphere as tundra soils warm. Conversely, increased plant growth under warming could remove C from the atmosphere and sequester it in plant biomass. Nutrient availability modulates ecosystem response to warming by influencing both plant growth and decomposition of soil organic matter, but the net effects of nutrient cycling on ecosystem C budgets are not well constrained. Phosphorus (P) is a limiting nutrient to plants and microorganisms in many ecosystems including the arctic. Soil minerals such as iron (Fe) oxyhydroxides strongly adsorb or co-precipitate with phosphate, the bioavailable form of P, but the potential for mineral-bound phosphate to limit P bioavailability has not been established for the organic-rich soils that dominate arctic tundra. Here, we characterized soil Fe and P species as a function of depth in the active layer (<30 cm) of low-centered and high-centered ice-wedge polygons at the Barrow Environmental Observatory on the Alaska North Slope. Our results demonstrate that Fe-bound phosphate is a large and ecologically relevant P reservoir in this system. Surface organic horizons were enriched in Fe and P relative to mineral horizons across all microtopographic features (trough, ridge, center). Soil Fe was dominated by organic-bound Fe and short-range ordered Fe oxyhydroxides, while soil P was primarily associated with oxides and organic matter in organic horizons but apatite and/or calcareous minerals in mineral horizons. Iron oxyhydroxides and Fe-bound phosphate were most enriched at the soil surface and decreased gradually with depth, and Fe-bound phosphate was more than four times greater than bioavailable water-soluble phosphate. These results are consistent with the observation that many tundra and boreal ecosystems exhibit accumulations of Fe oxyhydroxides and Fe-bound phosphate at presumed redox interfaces. However, the spatial and temporal variations in Fe-P interactions remain to be explored. We contend that Fe oxyhydroxides regulate phosphate solubility under fluctuating redox conditions in the arctic tundra and may serve as important controls on P bioavailability.

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Anaerobic Respiration Pathways and Response to Increased Substrate Availability of Arctic Tundra Soils

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The availability of labile organic carbon (C) compounds in Arctic tundra wetland soils is expected to increase due to thawing permafrost and increased fermentation as a result of decomposition of soil organic matter with warming. How microbial communities respond to this change will affect the balance of CO_2 and CH_4 emitted during anaerobic organic matter decomposition, and ultimately the net radiative forcing of greenhouse gas emissions from these soils. While soil water content limits aerobic respiration, the factors controlling methanogenesis and anaerobic respiration are poorly defined in suboxic Arctic soils. We conducted incubation experiments on two tundra soils from field sites on the Seward Peninsula, Alaska, with contrasting pH and geochemistry to determine the pathways of anaerobic microbial respiration and changes with increasing substrate availability upon warming. In incubation of soils from the circumneutral Teller site, the ratio of CO_2 to CH_4 dropped from 10 to < 2 after 60 days, indicating rapid depletion of alternative terminal electron acceptors (TEAs). Addition of acetate stimulated production of CO_2 and CH_4 in a nearly 1:1 ratio, which is indicative of methanogenesis. The composition of the microbial community shifted to favor clades capable of utilizing the added acetate such as the Fe(III)-reducing bacteria *Geobacter* and the methanogenic archaea *Methanosarcina*. In contrast, both CO_2 and CH_4 production declined with acetate addition during incubation of soils from the more acidic Council site, and fermentative microorganisms increased in abundance despite the high availability of fermentation products. These results demonstrate that the degree to which increasing substrate availability stimulates greenhouse gas production in tundra wetlands may vary widely depending on soil pH and geochemistry. Divergent soil biogeochemical conditions will mediate a range of possible pathways and fates for the abundant labile organic C released during permafrost thaw and thus influence radiative forcing of tundra soils.

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Timing and Duration of Hydrological Transitions in Arctic Polygonal Ground from Stable Water Isotopes

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The evolution of Arctic ecosystems in a changing climate will be strongly influenced by the temporal shifting of seasonal transitions and the cascading consequences of an earlier annual thaw and later annual freeze. The transition of the seasons in the Arctic are exceptionally abrupt and result in similarly abrupt landscape hydrological transitions as the landscape freezes and thaws with the seasons. Correspondingly, land surface models (LSMs) and earth system models (ESMs) that include Arctic landscapes must be able to capture these abrupt hydrological transitions that occur during the annual thaw and the deepening of the active layer. The goal of this work was to improve the representation of polygonal surface water hydrology to inform the development of process based LSMs and ESMs, particularly with respect to the timing and duration of hydrological transitions during the annual thaw. Daily surface water samples were collected from 11 locations across the Barrow Environmental Observatory and across arctic tundra morphologies (low centered polygon troughs, high centered polygon troughs, lakes, and drainages) during spring and summer of 2013. Stable water isotopes (δ^2H and δ^{18}O) were then used to appraise the hydrologically significant transitions at the Barrow Environmental Observatory (Utqiaġvik, Alaska) and relate them to shifts in the landscape energy balance, made apparent by the characteristic progression of physical changes during the annual thaw. Rayleigh fractionation models are used throughout to quantify the water balance in various hydrogeomorpologies characteristic of the Barrow Environmental Observatory.

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A Multi-Sensor Unoccupied Aerial System Improves Characterization of Vegetation Composition and Canopy Properties in the Arctic Tundra

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Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

Climate change can strongly influence vegetation distribution, structure, and function of terrestrial ecosystems, with potentially significant regional and global climate feedbacks. In the Arctic, climate is warming twice as fast as the global average, creating a complex mosaic of vegetation biophysical and landscape changes across the Arctic biome, including increased woody shrub cover, altered surface energy balance, and longer growing seasons. The heterogeneity of these vegetation responses requires new approaches capable of quantifying the fine- to larger-scale changes that are driving ecosystem-scale feedbacks. However, commonly used ground-based measurements are limited in spatial and temporal coverage, and differentiating low-lying tundra plant species is challenging with coarse-resolution satellite remote sensing. On the other hand, Unoccupied aerial systems (UASs) have the potential to fill this critical scaling gap between ground-based and satellite observations. To address this need, we developed a cost-effective multi-sensor UAS (the 'Osprey') using off-the-shelf instrumentation. The Osprey provides simultaneous collection of hyperspectral, optical, thermal, and structural data of vegetation canopies. We describe the deployment of the Osprey in the Arctic at our study site located in the Seward Peninsula, Alaska. A case study is presented to demonstrate the application of Osprey data products for characterizing the key biophysical properties of tundra vegetation canopies. We show that plant functional types (PFTs) representative of arctic tundra ecosystems were mapped with an overall accuracy of 87.4%. The Osprey image products identified significant differences in canopy-scale greenness, canopy height, and surface temperature among PFTs, with deciduous low to tall shrubs having the lowest canopy temperatures while non-vascular lichens had the warmest. The analysis of our hyperspectral data showed that variation in the fractional cover of deciduous low to tall shrubs was effectively characterized by Osprey reflectance measurements across the range of visible to near-infrared wavelengths. Therefore, the development and deployment of the Osprey UAS, as a

state-of-the-art methodology, has the potential to be widely used for characterizing tundra vegetation composition and canopy properties to improve our understanding of ecosystem dynamics in the Arctic, and to address scale issues between ground-based and airborne/satellite observations.

Reference

Yang D, R Meng, BD Morrison, A McMahon, W Hantson, DJ Hayes, AL Breen, VG Salmon, and SP Serbin. 2020. A multi-sensor unoccupied aerial system improves characterization of vegetation composition and canopy properties in the Arctic tundra. Remote Sensing 12: 2638. https://doi.org/10.3390/rs12162638

NGEE–TROPICS
NEXT-GENERATION ECOSYSTEM EXPERIMENTS–TROPICS

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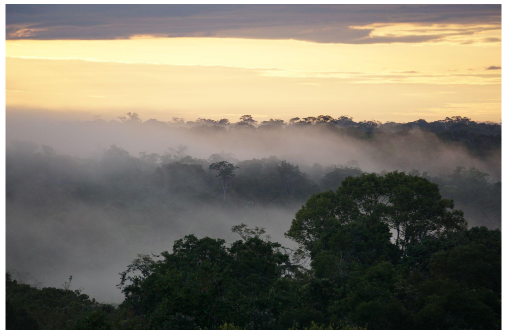


NGEE–Tropics
Poster Abstract Package
2021 ESS PI Meeting

ENVIRONMENTAL SYSTEM SCIENCE

Berkeley Lab · Brookhaven National Laboratory · Los Alamos National Laboratory · Oak Ridge National Laboratory · Pacific Northwest National Laboratory · CNRS · INPA Instituto Nacional de Pesquisas da Amazônia · NASA · NCAR · Smithsonian Tropical Research Institute · Forest Service

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

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Project: NGEE-Tropics

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Project Abstract: Tropical forests cycle more CO_2 and water than any other biome and are critical in determining Earth's energy balance. Yet processes controlling these tropical forest-atmosphere interactions that regulate the climate system are not well represented in the current generation of Earth system models (ESMs). In support of BER's mission to advance a predictive understanding of Earth's climate and environmental systems, the Next Generation Ecosystem Experiments (NGEE)-Tropics aims to deliver a greatly improved predictive understanding of tropical forests and Earth system feedbacks to changing environmental drivers over the 21st Century. A strong synthetic coupling of modeling and experiment-observational methods (ModEx) is the fundamental approach toward attaining this goal, with the grand deliverable a representative, process-rich tropical forest ecosystem model (the Functionally Assembled Terrestrial Ecosystem Simulator – FATES), extending from bedrock to the top of the vegetative canopy-atmosphere interface, in which the dynamics and feedbacks of tropical ecosystems in a changing climate can be modeled at the scale and resolution of a next generation E3SM grid cell. Phase 2 of NGEE-Tropics is structured around three Research Focus Areas (RFAs) that will advance understanding and model representation of tropical forest processes at the individual (RFA1), community to regional (RFA2), and regional and global (RFA3) scales in E3SM-FATES. Science activities within these RFAs are organized into ModEx Work Packages (WP). The WPs are coordinated to enable the delivery of RFA-level goals for FATES development and evaluation, and to apply FATES for addressing science questions at site to continental scales. This overview will highlight activities that synthesize across RFAs and WPs toward addressing integrative science questions.

Title: Data-model Fusion For Tree Community-scale Water Sourcing Depths In Tropical Forests

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Project: NGEE-Tropics

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Project Abstract: Diverse trees in the same forest may or may not be exposed to a drought depending on their water-sourcing depths. Estimating tree water-sourcing depths, or effective rooting depths (ERD), at the scale of the whole tree community is thus imperative to predict drought-induced mortality of a forest, but we are critically limited by data for ERD. This is especially challenging for tropical forests with hundreds of tree species and hundreds of thousands of trees.

We proposed a new data-model fusion approach, wherein data for water-sourcing depths for a functionally representative set of tree species in a forest informs a novel, community-scale model of ERD. The ERD model leverages commonly collected community-scale tree growth re-censuses and estimates the concurrent dynamics of water-availability vertically belowground to inversely estimate ERD. We successfully applied this approach as a proof-of-concept for 29 canopy tree species at Barro Colorado Island (BCI), Panama (Chitra-Tarak et al. *In Press*). Furthermore, this work highlighted that tree species whose water transport systems are considered more vulnerable to dehydration--based solely on their above-ground hydraulic traits--were, in fact, more buffered by deep-water access, experienced lesser drought exposure and had lower mortality rates across El-Nino droughts of a variety of intensity and duration.

Future work will involve MODEX development at multiple tropical sites validated with expanded measurements for ERD at BCI, Panama and new measurements at other intensively studied NGEE-Tropics sites, such as Manaus, Brazil, San Lorenzo, Panama and Luqillo, Puerto Rico, leveraging existing data for forest dynamics, hydrology and above-ground hydraulic traits. For ERD data estimates, we will use stable water isotopes as natural plant water source tracers. These leverage isotopic gradients due to evaporative enrichment of shallow soils vs. deep soil water to estimate ERD, when compared to the isotopic ratios of plant stem water. ERD will be determined by comparing isotopic composition of plant water with that of below ground water using established mixing models.

Publications:

Chitra-Tarak, Rutuja et al. “Hydraulically-vulnerable trees survive on deep-water access during droughts in a tropical forest.” *New Phytologist* (*In press*) [https://doi.org/10.1111/nph.17464].
Chitra-Tarak, Rutuja et al. “Soil Water Potentials (1990-2018) from a calibrated ELM- FATES, and rooting depth analyses scripts, PA-BCI, Panama. 2.0.” *NGEE-Tropics Data Collection.* (dataset). (2020) [http://dx.doi.org/10.15486/ngt/1696806]

Title: How Do Plant Hydraulic Traits Shape Species Demography and Distribution in a Wet Tropical Forest?

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BER Program: ESS

Project: NGEE-Tropics

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

Project Abstract: Climate change, including drought and warming temperatures, is impacting tropical forests around the world. This has implications for community dynamics, species' demography, and biogeochemical cycles. We investigated how species' hydraulic and drought response traits were associated with demography and regional distribution across a moisture gradient in tropical forests in Panama. We used long-term census data from Barro Colorado Island along with species occurrence data at 72 sites across the isthmus of Panama, and we collected species' archived trait data from the TRY Database, Xylem Functional Trait Database, NGEE-Tropics Data Archive, and other published sources. Focusing on evergreen species, we found a life history strategy trade-off, with species having high mortality rates, fast growth rates, and high recruitment rates on one end of the continuum, following a "live fast, die young" strategy. On the other end of the continuum were species with low mortality rates, slow growth rates, and low recruitment rates, following a "slow and steady" strategy. Xylem vulnerability to cavitation (P_{50}) was coordinated with these demographic trade-offs, as "live fast, die young" species had more vulnerable P_{50} and "slow and steady" species had more resistant P_{50}. Further, across 72 sites spanning a moisture availability gradient, wetter sites had higher photosynthetic rates and more vulnerable turgor loss point, while drier sites had lower photosynthetic rates and more resistant turgor loss point. These life history strategy trade-offs reveal how species' traits shape demography and distribution.

Title: An Improved Representation of the Effect of Photosynthesis on Stomatal Conductance Leads to More Stable Estimation of Conductance Parameters and Improves the Goodness-of-fit Across Diverse Datasets

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BER Program: ESS

Project: NGEE-Tropics

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

Project Abstract: Stomata play a key role in plants and forests by controlling the rates of transpiration and CO_2 diffusion between the leaf and the atmosphere. Modeling stomatal conductance (g_{sw}) is therefore essential to predict water and CO_2 exchange in plants and ecosystems. For given environmental conditions at the leaf surface (CO_2 concentration and vapor pressure deficit or relative humidity), models generally assume a linear relationship between stomatal conductance and photosynthetic CO_2 uptake (A), despite observations of a possibly nonlinear behavior. However, leaf level response curves of stomatal conductance to changes in photosynthesis are rare, particularly in the tropics, a factor which may have limited the study of this phenomenon. Here, we measured the response of g_{sw} and A to different irradiance spanning natural conditions from high irradiance to full dark in the leaves of six tropical species at different leaf phenological stages. We showed that the relationship between g_{sw} and A was non-linear, with a weak effect of increasing A on g_{sw} when A was low and a stronger effect when A was high. We reformulated the popular Unified Stomatal Optimization (USO) model to account for this phenomenon and to estimate the conductance parameters g_0 and g_1. This improved the goodness of fit and reduced bias in parameter estimates, resulting in a robust estimate for different irradiances. Previously undetectable relationships between conductance parameters and other leaf properties were revealed. The benefits of the nonlinear formulation were also demonstrated in data collected from attached and detached leaves, growth at ambient temperature and high CO_2, and various species from different environments. We propose that this empirical modification of the USO model can simplify data collection for parameterization and improve model performance in a wide range of applications. We also discuss the reasons for the nonlinearity in the g_{sw} response. We showed that a more complex conductance model based on the theoretical optimality framework does predict a nonlinearity at the transition between light-limiting and light-saturating photosynthetic rate. However, we also showed that the assumption on which optimality theory is based, that the marginal cost of water gain is constant, was not verified in our data, so that the more complex optimal models may not fully represent this phenomenon.

Title: Stem and Leaf Respiration in Tropical Ecosystems

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BER Program: ESS

Project: NGEE-Tropics

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

Project Abstract: Tropical forests fix more CO_2 than any other terrestrial ecosystem. However, they are also a major source of CO_2 through respiration (60GtC year^{-1}), several times more than anthropogenic emissions. High respiration rates constrain net primary productivity with estimates of carbon use efficiency (CUE) around 30% in the Amazon. For this project, we first described how autotrophic respiration is treated in the ecosystem dynamics model, Functionally Assembled Terrestrial Ecosystem Simulator (FATES). We then synthesize monthly stem growth and CO_2 efflux measurements from 80 trees in a diverse, tropical forest in the central Amazon. In addition, we analyzed real-time stem CO_2 efflux together with canopy temperature and sap velocity for 3 trees during the day and night. These two datasets were organized and shared in the Next Generation Ecosystem Experiments Tropics (NGEE-T) data archive. A positive linear correlation was found between stem growth rates and stem CO_2 efflux. CUE of stems was estimated as high as 80% for fast growing trees in the Amazon with 15 +/- 3% of carbon allocated to woody tissue released as CO_2. This compares favorably with the fraction of respiration per unit growth (11%) currently used in current ecosystem dynamics models, including the Functionally Assembled Terrestrial Ecosystem Simulator (FATES). Stem CO_2 efflux was suppressed by 10-50% during the day compared to the night demonstrating the importance of nighttime measurements. The results show high stem respiration rates are associated with high CUE of wood production during fast tree growth. We suggest future modelling and field observations should focus on quantifying maintenance (R_m) and growth (R_g) respiration of stems and how they vary with plant functional types (fast versus slow-growing), nutrient concentrations, environmental variables, and sapwood allometry.

Title: Tree Mortality Risk Factors in Tropical Forests

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BER Program: ESS

Project: NGEE-Tropics

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Project Abstract: Understanding the causes and consequences of tropical tree mortality is paramount to obtaining more accurate predictions of the future of tropical forests and the carbon cycle-climate feedbacks. Yet, the main mechanisms and pathways by which trees die remain unknown. This is especially problematic in the tropics, where the high levels of species diversity result in a variety of responses to the conditions to which the trees are exposed. We used 99,858 observations of tree-level conditions and subsequent survival of 31,203 trees of 1,977 tree species in 14 census intervals to estimate how conditions relate to survival. This study was conducted within six large-scale (24-50 ha) tropical forest plots of the ForestGEO network in the Neotropics (Amacayacu ,Colombia; Barro Colorado Island, Panamá) and Asia (Fushan, Taiwan; Huai Kha Khaeng, Thailand; Khao Chong, Thailand; Pasoh, Malaysia). We defined a condition as a risk factor for a species if it was associated with at least a two-fold increase in mortality, and quantified the prevalence, lethality, and contribution to total forest mortality of 19 risk factors. Besides the relatively well-known susceptibility of small, light-limited trees, we found trunk and crown damage were the conditions conferring the greatest risk of death. Other commonly studied risks such as those related to large tree size, liana infestation or herbivory were relatively less important at the forest level. Having a leaning trunk, or being defoliated constituted other important risk factors that have rarely been documented in tropical forests. We also found that the widely used modes of death (standing, broken, and uprooted) were not always associated with previously assigned mortality risk factors. Future research should focus on the links between these mortality risk factors, their climatic drivers, and the physiological mechanisms leading to tree death to help improve predictions of the future of tropical forests.

Title: Nutrient Cycling in FATES-ELM

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BER Program: ESS

Project: NGEE-Tropics

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

Project Abstract:Nitrogen and phosphorus play a critical role in growth and function of terrestrial ecosystems. Their availability in plants can limit tissue growth as well as modify physiological function. Incorporating the cycling of nitrogen and phosphorus into ecosystem models is an important step in estimating and/or predicting the evolution of terrestrial ecosystem structure and global carbon budget. Here we present the first version of fully coupled nitrogen and phosphorus dynamics between the Functionally Assembled Terrestrial Ecosystem Simulator (FATES) and the Energy Exascale Earth System Model (E3SM). This coupling enables 1) FATES plants to participate in competitive acquisition of nutrients in the soil with mineral surfaces (for phosphorus) and microbes, 2) impose mechanistic and conservative growth limitations on fates plants due to competitive uptake, and 3) return organic nitrogen and phosphorus to the decomposing litter pools. Here we describe and perform some verification of the model coupling.

Title: Linking Resource Availability to Pantropical Forest Response and Resilience to Cyclone Disturbance

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Project Abstract: Tropical cyclones have global environmental and socio-economic impacts, causing nearly $26 billion y^{-1} in damage. Because these disturbances are becoming stronger and occurring at higher latitudes in recent decades, understanding the mechanisms governing their influence on forest response (resistance) and resilience (pace of return to pre-disturbance values) is necessary. We conducted a meta-analysis to investigate the effect of soil resource availability, namely total soil phosphorus (P) concentration, on site-level forest response and resilience to cyclones pantropically. We evaluated cyclone-induced and post-cyclone litterfall mass ($g/m^2/day$) and P and nitrogen (N) fluxes ($mg/m^2/day$) and concentrations (mg/g), indicators of ecosystem function, and essential conduits for nutrient recycling in forest ecosystems. Across 73 case studies in Australia, Guadeloupe, Hawaii, Mexico, Puerto Rico, and Taiwan, total litterfall (sum of leaf, fine wood, reproductive and miscellaneous fractions) mass flux increased from ~2.5 ± 0.3 to 22.5 ± 3 $g/m^2/day$ due to cyclones. Individual mass flux responses varied from a negligible change in Taiwan with Haima to an instantaneous flux that was ~2 times the annual input in Bisley, Puerto Rico with Irma. Relative to pre-cyclone means, leaf litterfall P increased by 58.6 ± 2.3% and N concentration by 21.6 ± 1.2% after cyclones. Soil P and wind speed positively moderated immediate litterfall mass flux responses to cyclones. Total litterfall mass flux reached pre-disturbance levels within one year of the disturbance. Litterfall N and P concentrations remained higher than pre-disturbance levels during the same period. A significant interaction of soil P with time since the cyclone and gale wind duration best explained ($R^2 = 0.4$) the variability in the litterfall mass flux resilience. Our pantropical findings corroborate the prediction, based on single-site studies in Australia and Hawaii, that forests on low-P soils are less responsive and likely less resilient to cyclones than forests on high-P soils. Forest response in the face of intensifying cyclone disturbance will be determined, in part, by soil resource availability.

To further understand the forest resistance and resilience and associated carbon dynamics, we use ELM-FATES with cyclone-induced tree mortality (separated from other FATES mortality factors) added. We perform simulations with varied tree mortality fractions and find that both early and late-successional evergreen broadleaf forests respond to cyclone disturbance with total biomass reductions. Leaf biomass and leaf area index responds non-linearly to cyclones, suggesting a rapid closure of the canopy and fundamental needs of reasonable simulation of forest structure and biomass recovery following cyclones.

Title: FATES-SPITFIRE: Dynamic Ecosystem Assembly Through Interaction of Disturbance, Vegetation Strategies and Canopy Structure in the Tropics

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Project: NGEE-Tropics

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Project Abstract: For global scale simulation, a new axis of biogeography driven by fire disturbance is needed within Vegetation Demographic Models (VDM). Within the tropics, the location of forests and savannas are determined through the interaction of climate conditions, fire disturbance frequency and vegetation traits and state. Utilizing the Functionally Assembled Terrestrial Ecosystem Simulator (FATES), a size-structured VDM, with the fire behavior and effects module SPITFIRE, we explore thresholds of survival and resulting biogeography for simulations with trees that have contrasting fire tolerance traits and a C4 grass. Fire tolerance strategy is based on tree bark thickness, crown size and foliage resistance to heat, which are key fire-tolerance traits across woody plants. Within South America, observations demonstrate that trees within stable forest areas with traditionally low fire disturbance have thinner bark than trees in savanna areas that experience regular fire disturbance. SPITFIRE has been adapted within FATES to calculate scorch height at the plant level, to calculate grass fuel moisture based on climate, and to use spatially and temporally varying lightning ignitions. Simulations capture observed patterns for vegetation productivity, aboveground biomass and seasonal burned area for the recent historical period. Simulated biogeography of the fire-tolerant vs. -intolerant trees corresponds to observations of tree bark thickness variability across South America. Fire disturbance limits tree extent, with wetter, low disturbance areas retaining a higher stable tree fraction of the fire-intolerant tree. Transitional and drier areas with intermediate to high fire disturbance demonstrate dominance of trees or grasses conditional on fire frequency. Without fire, the fire-intolerant tree, which has lower wood density and thinner bark, is dominant and accumulates extensive biomass across the region. FATES-SPITFIRE tracks size-structured plant mortality and captures 'fire-trap' dynamics where fire-tolerant trees escape fire by achieving a canopy height above the flames or through fire resistant traits. These fire-vegetation feedbacks are critical for projection of ecosystem resilience and shifts under current and future conditions.

Title: Quantifying Spatial and Temporal Variation in Tropical Forest Canopy Disturbance Using Drone Photogrammetry

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Project: NGEE-Tropics

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

Project Abstract: Tree damage and mortality are important controls over carbon stocks and fluxes in tropical forests—these processes are also key uncertainties in current Earth system models. Tropical tree damage and mortality are currently uncertain because their rates are low, requiring frequent and large-scale observations to quantify variation, which is infeasible with labor-intensive traditional field methods. In this study, we used 3D drone photogrammetry to locate canopy disturbances from tree damage and mortality at ~ monthly (for 50 ha) and multiannual (for 1350 ha) intervals over 5 years on Barro Colorado Island (BCI), Panama. We found that on average approximately 2% of the forest is affected by canopy disturbance every year. Importantly, our data quantify high spatial and temporal variation in canopy disturbance rates. Spatially, disturbances occur more frequently on ridges, areas with high or low slope, older forests, and on certain geographic formations. Temporally, disturbance rates are positively associated with extreme precipitation events. Visual inspection of before and after drone imagery revealed that 23% of canopy disturbance (by area) is associated with tree damage (branchfalls), while the other 77% is associated with tree mortality (treefalls). Our results are relevant for improving mechanistic understanding of carbon cycling in this well-studied landscape, and for the representation of tree damage and mortality in ecosystem models.

Title: Coupled modeling of hillslope hydrology and ecosystem dynamics at Manaus and BCI

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BER Program: ESS

Project: NGEE-Tropics

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

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

Title: Gradients and Environmental Controls of Stem Number Density, Tree Height and Volume in the Brazilian Amazon Using Lidar Crown Detection

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BER Program: ESS

Project: NGEE-Tropics

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

Project Abstract: Tropical forests are critical to the function of the Earth system, but their tree size distribution is largely unknown because of the lack of systematic forest inventory that, in addition, limits the capabilities of satellites-based estimates (e.g. GEDI) as they critically rely on widespread reference observations. The size structure of forests is critical to demographic vegetation models such as FATES.As an alternative to ground inventory, we measure trees individually using high density airborne lidar data to estimate their structural properties by direct retrieval or through allometric models. We applied a lidar crown detection method to 470 randomly sampled airborne lidar plots (6.25ha each) collected in 2016 from a larger survey that randomly sampled terra *firme* forests across the entire Brazilian Amazon. For trees > 10 m tall, we calculated plot-level averaged values for stem number density (mean, 5^{th}-95^{th} percentile: 396, 281-509 trees ha^{-1}), average maximum tree height (43.9 m, 28.8-58.9 m), crown packing (19.7%, 9.2-26.8%) and basal area (28.2 m^2 ha^{-1}, 9.3-39 m^2 ha^{-1}). We found strong regional patterns with significant decreases in stem number density from northwest to northeast. In contrast, the gradient in tree height follows the opposite trend. The crown packing strongly decreases from northwest to southeast, whereas basal area follows a northeast-southwest gradient. Using a linear statistical model, we assessed environmental and disturbance controls (topography, soil fertility, forest fragmentation, climate, canopy-atmosphere interaction and climate stressors) on forest structure. We found that tree height and basal area are predominantly responses to topography and climate, crown packing is positively correlated with climate stressors (e.g. water deficit) and stem number density is also controlled by climate conditions. The explanatory power of the environmental factors is moderate and it varies when considering the entire Brazilian Amazon or regions individually. Our individual tree crown measurements represent a major advance to quantify the variability of the Amazon forest structure. While this approach does not replace detailed forest survey, it nonetheless provides consistent forest structure data where heretofore there was none.

Title: Tropical Forests and Emerging Hot Droughts

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Project: NGEE-Tropics

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

Project Abstract: Under a warmer climate, precipitation variation will interact with changes to surface air temperature and humidity to drive strongly increased VPD during droughts. Understanding the response of tropical forests to these hot droughts is critical to projecting ecosystem feedbacks to climate change. The 2015 drought represents an early indicator of these dynamics, as it showed strongly increased VPD as compared to previous droughts, and thus serves as an example of these emerging events. We will present results showing results from the 2015 drought in the Amazon, the timing of emergence of different VPD thresholds from CMIP6 models, and FATES simulations of physiological responses to these VPD anomalies.

ORNL's Terrestrial Ecosystem Science – Scientific Focus Area (TES SFA): a 2021 Overview

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Project: ORNL Terrestrial Ecosystem Science Scientific Focus Area (TES SFA)

Project Website: http://mnspruce.ornl.gov; http://tes-sfa.ornl.gov

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

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

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

Improving models of SPRUCE carbon cycling and phenology using observations

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Project: ORNL TES SFA

Project Website: http://mnspruce.ornl.gov; http://tes-sfa.ornl.gov

Project Abstract:
Uncertainty about land surface processes contributes to a large spread in model predictions about the magnitude and timing of climate change within the 21st century. Global peatlands are an important reservoir of carbon that may be at risk due to climate change and have not traditionally been well-represented in models, contributing to this prediction uncertainty. The Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment is applying whole-ecosystem warming and elevated CO_2 concentrations to an ombrotrophic bog in northern Minnesota to represent a range of possible future conditions and study the ecosystem responses. A version of the E3SM land model, ELM-SPRUCE, is under continuing development to predict the experimental responses and provide a framework for integration of wetland processes to Earth System models. ELM-SPRUCE is a peatland-specific of ELM including hummock-hollow microtopography, bog-specific hydrology, CH_4 cycling and Sphagnum moss dynamics, which were previously absent from ELM. Observations in the enclosures with warming treatments using phenology cameras indicated strong phenological responses to warming, the magnitude of which varies with species. We calibrate ELM-SPRUCE with observed phenology data, carbon fluxes, biomass and hydrology. The calibrated model is then subjected to the experimental treatments over 15-year period. We assess the fate of carbon stocks given the assumptions in ELM-SPRUCE, how this impacted by phenology, and strategies for reducing prediction uncertainty in the future.

Probing structural differences in contemporary soil carbon models

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BER Program: ESS

Project: ORNL TES SFA

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Project Abstract:
Hundreds of models have been developed to describe the formation and decomposition of soil organic carbon (SOC), representing different assumptions about the dominant processes governing SOC dynamics. Moreover, recent models employ even more complicated representations of microbial and mineral interactions, reflecting our evolving understanding of SOC. This has led to an explosion of potential SOC model configurations. Unsurprisingly, different process representations among existing models have led to divergent predictions about SOC responses to global change. As SOC models continue to evolve, there is a critical need to probe the drivers of this process-level uncertainty. Here, we investigate how alternative hypotheses affect predicted SOC responses to altered carbon inputs—which are changing due to multiple environmental and anthropogenic drivers. We developed a generalizable SOC model within the multi-assumption architecture and testbed (MAAT)—a modular modeling code that can easily vary model process representations. We evaluated how alternative hypotheses about microbial constraints and mineral saturation shape SOC responses to altered input rates. Then, we integrated contemporary microbially explicit SOC models (e.g. MIMICS, MEND, CORPSE) into MAAT to uncover the sources of process-level inter-model variability. Using a simple three-pool model, we find that model assumptions about microbial constraints and mineral saturation exert substantial control over the trajectory of SOC responses to altered input rates. Representing alternative hypotheses about constraints on microbial growth, lifespan, and mineral-associated SOC capacity led to linearly increasing, non-linearly increasing, or unresponsive SOC trajectories. More complicated, contemporary SOC models also predict substantially different SOC responses ranging from complete insensitivity of SOC to input rates to linear relationships. We find that unifying the representation of key processes brings model predictions into alignment. For example, representing microbial density-dependence in MEND leads to predictions that more closely mirror other models (e.g. MIMCS). We will discuss how these analyses are informing further developments of our multi-assumption SOC model and how this multi-assumption approach will be critical in efficiently directing future empirical studies and model development.

Nitrogen and Phosphorus Cycling at SPRUCE: Warming increases availability of crucial limiting nutrients

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BER Program: ESS

Project: ORNL TES SFA

Project Website: https://tes-sfa.ornl.gov/, https://mnspruce.ornl.gov/

Project Abstract:
Slow decomposition and isolation from groundwater mean that ombrotrophic peatlands store a large amount of soil carbon (C) but plant growth is constrained by the low availability of nitrogen (N) and phosphorus (P). To better understand the role these limiting nutrients play in determining the C balance of peatland ecosystems, we compiled comprehensive pretreatment N and P budgets for the S1 Bog (Salmon et al, 2021) and documented changes in N and P availability following the implementation of whole ecosystem warming treatments at SPRUCE. Pretreatment nutrient budgets showed that N accumulates in the bog ecosystem at 0.2 ± 0.1 g N m^{-2} y^{-1} while annual P inputs were generally balanced by losses from the bog ecosystem. Plant functional types (PFTs) varied in their degrees of N versus P limitation, allocation across tissues, and internal recycling of N and P. Building on these pre-treatment measurements, we used ion-exchange resins to investigate the seasonal and annual effects of warming and elevated [CO_2] on plant-available N and P in the SPRUCE enclosures. We found that warming increased resin-available NH_4-N and PO_4-P at similar rates, but the magnitude of the response increased over time and varied across the highly heterogeneous bog surface and with peat depth. In recent years, we observed a large increase in resin-available N and P in surface peat that was inversely related to the warming-induced decline of *Sphagnum* nutrient requirements. The ELM-SPRUCE terrestrial biosphere model captured N pools and fluxes better than P when simulating pre-treatment conditions. In response to warming, however, the model tended to underestimate the increase in plant-available nutrients, especially in deeper peat. ELM-SPRUCE predictions of peatland nutrient cycling under climate change scenarios must therefore account for the initial distribution of N and P across peatland soil and vegetation pools as well as the interplay between vegetation nutrient acquisition and microbial activity across microtopography and depth. Together, our pre- and post-treatment analyses highlight the role that N and P cycling play in: (1) determining ecosystem structure and function and (2) advancing our ability to predict the C balance of warming peatland ecosystems.

Belowground Plant Trait Strategies Across The World

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Project: ORNL TES SFA

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Project Abstract:
Land plants have developed diverse strategies to acquire soil resources for over 400 million years, but only recently have we started to comprehend the ecosystem-scale consequences of belowground plant trait strategies and their response to changing environmental conditions. In peatlands, one of the planet's most carbon-dense ecosystems, warming increases the length of ericaceous shrub roots by as much as 130% per °C. In turn, warmer peat temperatures are associated with increased abundance of fungal rhizomorphs and lengthening of the belowground active season. Taken together, these changes may affect peatland ability to store carbon into the future. Current investigations of plant-fungal interactions at the SPRUCE experiment show that plants rely on both their fine roots and symbionts for resource acquisition and that warming heighten their reliance on fine roots. These results will further our understanding of belowground acquisition strategies effects on carbon dynamics in peatlands. At the global scale, the Fine-Root Ecology Database (FRED) has been at the forefront of efforts to fill gaps in our understanding of belowground trait variation. Results from our team and international collaborations have revealed species-specific tradeoffs in mycorrhizal association and root traits as well as linkages within and among above- and belowground plant traits. In addition, we have released a third version of FRED that now includes a searchable interface so that scientists may filter more than 150,000 root trait observations according to their interests. Furthermore, we continue to harvest data from underrepresented tundra and tropical ecosystems. Site-specific observations of rooting distribution and dynamics in response to changing environmental conditions at SPRUCE, along with a global perspective provided by FRED, are serving as the foundation to improve the representation of fine-root form and function in the E3SM Land Model.

Plant Physiological Response to Whole Ecosystem Warming and Elevated CO_2

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Project Website: https://tes-sfa.ornl.gov/, https://mnspruce.ornl.gov/

Project Abstract:
Climate warming has an outsized impact on boreal and arctic biomes, with significant implications for ecosystem carbon uptake and atmospheric feedbacks. At the southern edge of the boreal forest large, open-topped enclosures are exposing a natural peatland to whole-ecosystem warming × CO_2 enrichment (https://mnspruce.ornl.gov/). After only a few years of warming and CO_2 treatments, the plant community in this bog ecosystem is showing signs of stress with crown damage, branch tip dieback and even mortality in the conifer species: the deciduous *Larix laricina* and evergreen *Picea mariana.* Similar results have been exhibited by the woody shrubs, *Chamaedaphne calyculata* and *Rhododendron groenlandicum*, which incidentally are also experiencing increased herbivory with warming. We examined the mechanisms of the hydraulic damage, hypothesizing that, even in this ecosystem characterized by saturated soils, evaporative demand created by elevated temperatures could exert critical tension on the hydraulic system, leading to dysfunction in the xylem.

We found increased vapor pressure deficient, driven by air temperature, translated into greater plant water stress. Interestingly, diurnal water potential patterns revealed contrasting hydraulic strategies in the two tree species, with *Picea* operating conservatively, below its turgor loss point, while *Larix* operated at or above its turgor loss point, increasing water use with warming. Despite the divergence in water stress patterns, both species experienced a significant increase in hydraulic dysfunction with warming, measured as an increase in native xylem embolism. Using microscopy, we also assessed xylem area, ring width, lumen area and density – characteristics linked to hydraulic function. While there was large variability in growth ring width response to warming, elevated CO_2 + warming resulted in a significant increase in xylem wood production in branches, which can facilitate greater water movement though the stem.

Together our results show that elevated evaporative demand can strain plant hydraulic systems even in regions not at risk of severe soil water limitation. But there is some evidence that warming stress may be offset by increased CO_2, which can both increase availability of non-structural carbohydrates and reduce water stress. Now in our sixth year of treatments, we continue to track changes in hydraulic responses to understand what acclimation mechanisms plants may leverage to overcome the severe heat/water stress imposed by the treatments.

Root Function - Process-Level Studies Focused on Mycorrhizae, Drought, Temperature and Neutron Imaging

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Project: ORNL TES SFA

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Project Abstract:
Assessment of root function is extremely difficult, but new field techniques and advances in imaging technology are allowing unprecedented insight into root dynamics. Neutron imaging is highly sensitive to hydrogen ions, thus biological material and water are readily visible, which allows for *in situ* assessment of root structure, root growth, root water uptake & internal root water transport. Results with various woody plants, maize and switchgrass indicate significant variability in water dynamics across the soil-rhizosphere-root pathway, including root water uptake and hydraulic redistribution, hysteresis in water release curves and soil wettability. Measured root water extraction rates by cottonwood ranged from 0.003 to 0.02 g cm^{-2} h^{-1}, with lower rates for larger roots. Across species, root rhizosphere development increases with root size, stabilizing as roots reach ~2 mm in diameter, likely linked to their suberization. Neutron radiography has also indicated significant root and mycorrhizal impacts on soil hydraulic parameters, including hydraulic conductivity and residual water content. Presence of mycorrhizae led to more even water extraction rates in soil areas with and without roots, as well as increased shoot:root ratio. Results are important for testing and improving models of root water uptake and its linkages to root traits – one easy model improvement is to use root biomass as a modifier of hydraulic parameters. Other key root processes that models are sensitive to include dynamics of root carbon allocation, relationships between roots and mycorrhizal fungi, root nutrient uptake, and root respiration and acclimation to temperature. In poplar exposed to two levels of warming, photosynthetic acclimation and biomass increased for both treatments, whereas belowground, peak biomass was achieved by the intermediate treatment, and root respiration suppressed at the highest temperature. Respiration rates of intact root systems of mature trees increased their contribution to total soil CO_2 efflux with warming, particularly for acquisitive root strategies, as represented by root functional trait space axes related to high specific root length, high root tip abundance, and low root tissue density Here, we leverage field and chamber-based neutron imaging techniques to assess root functional dynamics *in situ*, particularly patterns of water uptake and respiration linked to species and root traits. We also

discuss current and future improvements in neutron imaging analysis and application to belowground systems.

The Missouri Ozark AmeriFlux Site: An Ecosystem Observatory Enabling Improved Understanding of Drought Impacts on Deciduous Forests

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The Missouri Ozark AmeriFlux (MOFLUX) site was established in 2004 in the Ozark Border Region of Central Missouri. The site is located in a *Quercus-Carya* forest, and high precipitation variability induces frequent physiological drought stress, a situation that is often is exacerbated by the comparatively thin soils. MOFLUX (AmeriFlux ID, US-MOz) is instrumented to monitor processes from roots-to-shoots and leaf-to-landscape. It is based around a tower that is equipped for observing ecosystem fluxes using the eddy covariance technique, and more recently, canopy scale sun-induced chlorophyll fluorescence (SIF). In addition to the extensive suite of automated instrumentation, routine biometric and ecophysiological data, including weekly to biweekly measurements of community predawn leaf water potential (Ψ_{leaf}) are collected. MOFLUX has evolving scientific objectives driven by ever-deepening understandings of ecosystem processes. However, the core ecosystem flux and supporting datasets provide an invaluable long-term perspective on how drought dynamics and extreme events shape the function and structure of temperate deciduous forests and are essential for developing and testing ecosystem models. Here, we provide an overview of the MOFLUX site and highlight the science enabled by novel long-term observations and current ongoing science activities. Specifically, we will report the following:

- We conducted novel analyses leveraging coordinated Ψ_{leaf} and ecosystem gas exchange observations. First, we synthesized Ψ_{leaf} (predawn and mid-day) with ecosystem gas exchange to estimate the ecosystem scale hydraulic conductance (K_{eco}). K_{eco} represents a significant constraint on ecosystem transpiration and gross primary productivity that increases during drought. In a separate analysis, we used community predawn Ψ_{leaf} and evapotranspiration observations during a major drought to deduce an ecosystem scale wilting point. The ecosystem wilting point is an ecosystem property tightly related to drought responses, and results imply canopy traits governing wilting are coordinated with root system traits and soil characteristics.
- We developed a three-way carbon dioxide flux-partitioning algorithm that separates net ecosystem exchange into above-ground plant respiration, below-ground root and soil

respiration, and gross primary production. We found that on annual time scale, belowground soil respiration dominates over aboveground plant respiration in total ecosystem respiration but the relative contributions of different sources vary seasonally.

- Current research activities include an increased emphasis on connections between above and belowground processes, on observing and interpreting canopy SIF to enable improved scientific understanding of ecosystem physiology, and on developing an integrated model of photophysics, photochemistry and biochemistry of photosynthesis for applications in ecosystem models.

Changes in Soil Microbial Community and Function with Changes in Soil Moisture and Texture

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Project: ORNL TES SFA

Project Website: https://tes-sfa.ornl.gov/

Project Abstract:
Soil microbes are very sensitive to soil moisture, but there are many reasons to explain observed changes in CO_2 fluxes. Generally, at lower soil moisture, CO_2 emissions decrease, which could be attributed to changes in substrate availability, soil microbial biomass and community composition, microbial dormancy, and enzyme activity. Under transient (wetting-drying) conditions, breaking of soil aggregates can alter substrate availability, microbial community composition can change, and microbes can protect themselves from death through osmolyte (metabolite) production. Here, a set of lab incubations involving 3 different soil textures (sandy, loamy, and clayey soils) were conducted over a range of soil moistures and over steady-state and transient conditions. The steady state moisture manipulation showed different moisture optima for highest microbial respiration for different textured soils. Extractable organic carbon was greatest under dry conditions, and carbon degrading enzyme activity was lowest, indicating lower microbial activities for all soil textures. The transient incubation experiment sought to understand mechanisms fueling the “Birch effect”, by comparing soils that were air-dried and at water holding capacity, under both steady-state (55% water holding capacity) and transient conditions. We found higher cumulative soil organic carbon loss under transient moisture state compared to steady state, and that different mechanisms contributed to the Birch effect in different textured soils. In sandy soil, metabolite accumulation and changes in bacterial community structure were the most important Birch effect responses; while in loamy and clayey soils, metabolite accumulation and release of aggregate protected carbon were more important. Therefore, the response of microbial respiration to changing soil moisture will strongly depend on the sensitivity to textural differences. Finally, a field-scale moisture manipulation experiment – drought, rainfed, and irrigated – in a soybean field in western Tennessee showed decreases in CO_2 emissions and enzyme activity concomitant with increases in microbial biomass and extractable organic carbon under the imposed drought compared to rainfed and irrigated conditions. This likely suggests increased microbial dormancy and substrate accumulation under drought conditions, which may fuel CO_2 emissions upon rewetting. This comprehensive set of

analyses provides key information on how microbes respond to changes in moisture as a function of soil texture, under both steady state and transient conditions, and ranging from lab to field scales.

River Corridor Hydrobiogeochemistry from Reaction to Basin Scale

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

Project Abstract: *The Pacific Northwest National Laboratory (PNNL) River Corridor Science Focus Area (RCSFA) is transforming understanding of spatial and temporal dynamics of coupled hydrologic and biogeochemical processes in river corridors from reaction to watershed and basin scales, thus enabling mechanistic representation of river corridor processes and their response to disturbances in multiscale models.* Rivers are integrators of watershed processes as their composition and dynamics reflect conditions in the surrounding landscapes and subsurface environments. Hydrologic exchange flows (HEFs) between river channels and surrounding sediments are a ubiquitous feature of river corridors but vary substantially in their character and impacts. HEFs are known to promote enhanced hydrobiogeochemical function in river corridors, yet we lack transferable understanding of how their governing processes vary through space, time, and across scales and watershed settings. Furthermore, the representation of river corridors in basin-scale integrated land surface models is currently limited, and their cumulative impacts on watershed function are poorly understood. Accordingly, it is difficult to predict how river corridor hydrobiogeochemistry will respond to future disturbances. Our team is developing mechanistic understanding of the processes that link hydrologic, geochemical, and microbial processes in river corridors and integrating that new knowledge into numerical models at scales from fundamental reactions to major river basins to enable robust prediction. Wildfires and the compounding effects of precipitation events are key disturbances that influence river corridor hydrobiogeochemistry and are prevalent in the Columbia River Basin (CRB) and its constituent watersheds. To elucidate the impacts of spatial and temporal variability of hydrobiogeochemical processes across scales, as perturbed by wildfire disturbances, we are performing integrated field, laboratory and modeling studies in the Yakima River Basin (YRB), a major watershed that includes a wide ranges of stream orders and all major watershed classes in the CRB from forested mountains to shrub-steppe desert lowlands. Prediction is focused on elemental (C, N, P) cycling and key water quality variables including temperature and contaminants such as nitrate. We are using a distributed, open science approach based on our successful development of WHONDRS to develop regional and national partnerships that will underpin this research. A multiscale ModEx approach integrates process-based and data-driven models with experiments and observations across reaction to basin scales in coupled iterative learning cycles. Connecting project outcomes to the efforts of other agencies will enable robust watershed predictions to facilitate the solution of national challenges in water quality/quantity and Earth System prediction.

Modeling Coupled Organic Matter and Nitrogen Cycling in River Corridors Across the Columbia River Basin

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Project Abstract: *This element of the PNNL SFA seeks to quantify the cumulative impacts of river corridor hydrologic exchange flows (HEFs), dissolved organic matter (DOM) chemistry, and microbial activity on biogeochemical cycling, water quality, and contaminant mobility across the Columbia River Basin (CRB) under both baseline and disturbance conditions.* River corridors play important roles in organic matter and nitrogen cycling and removal of excess nutrients. At basin scales, the incorporation of hydrologic connectivity and molecular information on microbiome structure (i.e., species composition and distribution of enzyme-encoding genes), microbial expression, and metabolomes will greatly improve a river corridor model (RCM) in capturing distinct water quality signatures in connection to variations in land use, hydrogeology, climate, and disturbances. We have developed an RCM that resolves reactions occurring in both the water columns and in the river corridors as impacted by the hydrologic exchange flows (HEFs). Applying this RCM to the Columbia River Basin (CRB), we found that the physical properties influencing HEFs and land use are the primary controls of the spatial variability in river corridor denitrification. We have also developed integrated watershed models leveraging the IDEAS-Watersheds software ecosystem to understand terrestrial inputs to river corridors through both surface and subsurface pathways under baseline and disturbance conditions. Machine learning methods have been applied to integrate data from USGS river gauges and remote sensing to improve model parameterization and calibration. Next, we will enhance the mechanistic foundation of the RCM by linking dynamic river flow processes and heterogeneous terrestrial inputs with variable temperatures and reaction kinetics (informed by molecular properties) to investigate water, energy, and solute fluxes across the river-groundwater interface under both baseline and post-fire conditions. Stream and riverbed temperature regimes simulated by the model can also be used to map thermal refugia for resilient aquatic habitat. Our approach can be generalized beyond CRB and applied to other basins facing environmental disturbances and water challenges of national significance.

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

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

Project Abstract: *This element of the PNNL River Corridor SFA seeks to identify places/times across the Yakima River Basin (YRB) in which sediment-associated metabolism strongly influences active channel biogeochemistry, and reveal drivers of underlying molecular properties.* To represent processes governing river corridor biogeochemistry in predictive models, we need to understand how and why biogeochemical contributions from sediment-associated organisms vary through space/time; such contributions vary from 3-96% of respiration. Recent RCSFA work predicts spatial variation in sediment contributions to respiration. To evaluate these predictions, we are using dissolved oxygen sensors across 2nd-7th order streams in the YRB. Site locations were selected using a multi-iteration ModEx approach. The team identified system features that had the strongest influence over model predictions of river corridor hydrology and biogeochemical rates (e.g., aerobic respiration and denitrification). These model-relevant features were then used to parse the YRB into different classes using machine learning algorithms. In turn, field sites were selected to span the identified classes while accounting for logistical constraints inherent to *in situ* sensor deployments (e.g., land ownership). The full set of selected sites span four sub-basins in the YRB and are distributed across two complementary efforts that each focus on longer time series (multiple months) or spatial variation at a shorter time scale (1 week). The temporal component includes six sites distributed across stream orders and biomes from low order montane settings to high order lowland river settings and coincide with other agencies' gauging installations. The spatial component includes ~28 sites distributed more broadly across the YRB to maximize environmental breadth and provide opportunities to evaluate common patterns and context dependencies. Outcomes of the sensor deployments will be compared to model predictions for the contributions of sediments to river corridor respiration. Deviations between observations and model predictions will be studied to help guide model refinements through modifications to process representations and/or parameterizations. Sensor deployments are awaiting permit approvals and to provide longer-term context and model-relevant data, the model and measurement teams worked together to identify water chemistry variables most important for model evaluation. Selected variables span standard measurements (e.g., organic C concentration, ion chemistry, carbonate/bicarbonate speciation) and less standard measurements (e.g., FTICR mass spectrometry), all of which can be used to drive and/or evaluate reaction networks in the dynamic basin-scale models used by the SFA. Water chemistry samples are currently collected weekly at the six temporal study locations.

The Impacts of Wildfire Disturbance on Hydrobiogeochemical Function

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Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: ESS
Project: PNNL River Corridor SFA (RCSFA)
Project Website: https://www.pnnl.gov/projects/river-corridor

Project Abstract: *This element of the RCSFA aims to reveal the mechanisms by which wildfires impact biogeochemical cycling in river corridors from reaction to basin scale. We aim to further improve model predictive capacity in watersheds impacted by fire disturbances, important for ascertaining the influence of fire on ecosystem structure and function*. We have recently completed a modeling experiment to evaluate pyrogenic organic matter (PyOM) bioavailability, leveraging a model developed by the RCSFA that uses OM stoichiometry to predict aerobic respiration. The predicted bioavailability for a diversity of literature derived PyOM compounds is comparable to natural OM (NOM) pools in global surface waters and sediments. However, the model-derived carbon use efficiency of PyOM varied dramatically, indicating a large range in PyOM's impact on ecosystem function. For instance, phenolic PyOM and 'Black Carbon' ('BC') molecules had lower metabolic efficiency than other PyOM and NOM compounds, and 'BC' metabolism was also less negatively impacted by oxygen limitation. This work supports current theories that PyOM is more bioavailable than traditionally accepted, supporting growing evidence that it may be an underappreciated driver of river corridor biogeochemistry. Building upon this modeling exercise, we have implemented a large-scale burn severity experiment to identify the impacts of differing burn severities on NOM chemistry. These experiments are focused on recreating fire conditions that will result in analogous burn severities to those observed in the natural environment. This modeling and experimental work is complemented by several ongoing field campaigns, aimed at developing an understanding of the temporal trajectories of wildfire impacts, and relating pyrogenic impacts to watershed features. We have established in-fire and out-of-fire reference sites in the Yakima River Basin – in the 2020 Cold Creek Fire and Evans Canyon Fire burn perimeters – and have sampled surface waters routinely since December 2020. We also highlight the spatiotemporal trends in storm response of five streams spanning a range of landscape characteristics and burn severity impacted by the 2020 Holiday Farm Fire, which burned >700 km^2 of forest in the Willamette River Basin, in collaboration with the Eugene Water and Electric Board (EWEB). We complement EWEB's water quality monitoring efforts by focusing on shifts in dissolved organic matter (DOM) quality during the first storm events following the fire. Hourly sampling during the storms revealed stream-specific responses in the magnitude and timing of DOM concentrations and quality, highlighting a differential response of each stream which overprint the temporal trends in immediate post-fire storm responses.

Hydrobiogeochemical Features and Function Across Basins

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

Project Abstract: *This element of the PNNL River Corridor SFA combines WHONDRS data and numerical modeling to provide transferable principles that integrate organic matter (OM) chemistry, microbial gene expression, biogeochemistry, and disturbance.* We extend the RCSFA to the globe using crowdsourcing to understand transferable principles and to further establish ESS as a global leader in open watershed science. We are leveraging WHONDRS data while shifting the sampling paradigm to efforts guided more directly by the community. New sampling campaigns are smaller than previous global efforts and emphasize environmental contrasts. For example, samples are being taken through time in an agricultural stream system across different hydrologic conditions. This leverages existing research studying stream hydrobiogeochemistry. In another instance, we partnered with EXCHANGE (WHONDRS-like part of COMPASS) and the University of Quebec to study OM chemistry from source to sea along the St. Lawrence River. This spans multiple environmental gradients and a long-term research program. There are many more sampling efforts, including expansion to additional continents such as Africa. We also continue to generate data from existing samples such as metagenomics via JGI. These data are part of the Genome Resolved Open Watersheds (GROW) database. GROW goes beyond the RCSFA and is an open resource for global river corridor genomics. WHONDRS data are also increasingly used to gain new hydrobiogeochemical insights. For example, Danczak et al. (2021) discovered 'thermodynamic redundancy' whereby OM thermodynamics are invariant despite changes in molecular composition of OM. Changes in the identity of organic molecules may not, therefore, translate into functional differences associated with thermodynamics. In a community-led paper, Mueller et al. (2021) showed a strong influence of natural OM over transformations of organic contaminants. Garayburu-Caruso et al. (2020) provided a global summary of OM chemogeography across surface water and sediments. They found continental-scale gradients in OM chemistry, indicating large scale drivers of chemical properties. We are also changing the paradigm of open science through global crowdsourcing using WHONDRS data to study OM chemistry. Crowdsourcing in this effort spans the entire research life cycle and due to a high level of interest, will be a special issue of crowdsourced manuscripts all using WHONDRS data. Another outreach effort is launching the ICON Science institute, in partnership with EXCHANGE and GROW. The institute, launching in summer 2021, will enable the use of ICON principles across all of science.

Hydro-Biogeochemical Reactivity of Subsurface Interfaces
SLAC Floodplain Hydro-Biogeochemistry SFA Project Overview

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BER Program: ESS

Project: SLAC Floodplain Hydro-Biogeochemistry SFA

Project Website: https://www-ssrl.slac.stanford.edu/sfa/

Project Abstract: Floodplains are large, hydrologically active landforms, enriched in organic carbon and containing abundant and diverse microbial communities. Subsurface interfaces within floodplains are extensive, and exhibit sharp redox and solute contentration gradients that support intense biogeochemical cycling of carbon, metal micronutrients (*e.g.*, Fe, Mn), and other solutes. The biogeochemical function of subsurface interfaces is controlled by intricate coupling between hydrological and biogeochemical processes. Yet, in spite of their importance, *our understanding of subsurface interfaces as nexuses of hydrological and biogeochemical process coupling is poor*.

The mission of the SLAC Floodplain Hydro-Biogeochemistry SFA is to develop conceptual and numerical process representations to describe the coupling between hydrological, biological, and geochemical (*i.e.,* "hydro-biogeochemical") processes across subsurface interfaces in response to hydrologic perturbations such as onset of spring flooding and summer drought. To do so, we are studying: (i) meter-scale hydrological exchange flows and cm-scale ion transport across subsurface interfaces; (ii) changes in microbial community structure and diversity; and (iii) the molecular/electronic structures and reactivity of organic carbon- and iron-bearing colloids, which are exported across interfaces. These factors interact across spatial and temporal scales to produce biogeochemical hot spots and hot moments. We are accomplishing this program through integration of field observations and sampling, laboratory experiments, and hydrological and reactive transport modeling that contributes to IDEAS-Watersheds and the ESS modeling ecosystem.

We are focusing on two important types of interfaces that are abundant in floodplains, but which have received little research attention at molecular-to-system levels: (1) Interfaces between gravel bed alluvium and overlying organic- and metal-enriched soils, which are ubiquitous across the intermountain West, as exemplified by our field sites at Slate River, CO and Riverton, WY; (2) interfaces surrounding fine-grained sediment lenses embedded within coarse-grained aquifer material, which promote the establishment of reducing conditions in surrounding coarse and otherwise oxic aquifer material, altering groundwater compositions. This work is providing new and deeper mechanistic process representations of hydro-biogeochemical coupling within floodplains, their impact on water composition, and their responses to perturbations.

SLAC Floodplain Hydro-Biogeochemistry SFA: Reactivity, Structure, and Transport of Colloids and Particles Across Subsurface Interfaces

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BER Program: ESS

Project: SLAC Floodplain Hydro-Biogeochemistry SFA

Project Website: https://www-ssrl.slac.stanford.edu/sfa/

Project Abstract: Floodplains characteristically exhibit a multitude of juxtaposed soil layers with sharply contrasting physicochemical and hydrologic properties. Water movement across interfaces between these layers results in mixing of porewaters of distinctly different chemical compositions, stimulating a host of biogeochemical processes, including the production of colloids (operationally defined here as >0.15 µm). Field observations from our Slate River, CO, field site show that Fe- and organic C-rich colloids form in fine-grained, primarily anoxic soils when oxic water from the gravel bed penetrates into the finer layers, and subsequently can be exported back across this interface when groundwater flow direction changes. Independently, laboratory observations using soils and sediments from our Riverton, WY, field site indicate that fine-grained, anoxic zones release colloids or particles such as active bacterial cells with substrates that stimulate the spread of reducing conditions into proximal coarse-grained zones. Thus, we hypothesized that colloidal transport across subsurface fine-anoxic and coarse-oxic interfaces drive downgradient biogeochemical reactions.

We have tested (and continue to test) this hypothesis through a suite of laboratory column and incubation experiments, coupled with reactive transport modeling. In addition, we are investigating the structure and composition of colloidal exports from fine-grained to coarse-grained zones and their stability, reactivity, interactions with the coarse-grained matrix, and transport properties. In the past year, we have discovered that the ratios of sulfide to initial Fe(III) and final Fe(II) to Fe(III) are key controlling factors for the size and stability of colloids forming in sulfidic zones. Further, our iterative coupling of laboratory experiments and reactive transport modeling has provided quantitative evidence that particulate/colloidal organic matter exports most likely include live microbial cells. Because these exports include active enzymes that facilitate the establishment of reducing reaction networks in an otherwise oxic environment, they constitute *exported reactivity*. These findings demonstrate that knowledge of the composition of material exchanges (solutes, colloids, particles, microbes) and their impact on biogeochemical reaction networks on both sides of the interfaces is critical for predicting larger-scale environmental processes (*e.g.*, greenhouse gas emissions, contaminant transport to ground- and surface waters).

SLAC Floodplain Hydro-Biogeochemistry SFA: Hydro-Biogeochemical Reactivity Across Interfaces in Riparian Floodplains Along Slate River, CO

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BER Program: ESS

Project: SLAC Floodplain Hydro-Biogeochemistry SFA

Project Website: https://www-ssrl.slac.stanford.edu/sfa/

Project Abstract: Interfaces between conductive gravel bed alluvium and overlying nutrient- and metal-enriched soils are ubiquitous in riparian environments of the intermountain West. These interfaces are laterally extensive zones where sharp redox gradients and intense microbial activity may substantially alter watershed-scale nutrient and metal micronutrient / contaminant availability. The biogeochemical function of these interfaces is controlled by intricate coupling between hydrological and biogeochemical processes. Yet, this coupling is poorly understood.

We investigated the relationship between hydrological transitions and biogeochemical responses in a representative riparian floodplain along the Slate River, Gunnison County, CO. Beaver dam construction adjacent to this site induced a massive hydrological perturbation in September 2019. Field measurements and hydrological modeling suggest that the onset of ponding and partial inundation reversed both horizontal and vertical flow directions in the shallow ($\leq$ 2 m) soils, leading to greatly increased downward infiltration of iron-rich *anoxic* porewater into the underlying gravel bed. In contrast, measurements and simulations suggest that, prior to dam construction, evapotranspiration (ET)-driven upward flow carried *oxic* water from the gravel bed into the overlying soil. A new site hydrologic model predicts that the hydrologic shift created an oxygen minimum zone ($<$ 1 mg/L) that is controlled by the balance between oxygen penetration and microbial respiration.

The increase in anoxic porewater adjacent to ponded sites is reflected in microbial community structure and diversity. For example, methanogenic archaea and sulfate-reducing bacteria are more abundant in these soils relative to their non-flooded counterparts. These observations imply significant changes in microbially-mediated biogeochemical cycling in soils impacted by flow reversal. We conclude that prolonged surface water impoundment and attendant increases in adjacent groundwater levels alter groundwater and nutrient flow vectors and fluxes, leading to redox zonation of the floodplain. Our model predicts that, proximal to ponded water, anoxic porewater and stable microbial communities persist. Enhanced downward export of anoxic porewater and nutrients into the conductive gravel bed occurs. Further from the river, the “distal zone”, where seasonal cycles dominate (as opposed to inundation), is influenced by ET and lateral recharge from inundated regions. Enhanced upward transport of oxic gravel bed groundwater into overlying anoxic soils also occurs in this zone. Our 2021 field program is focused on defining the boundary between these zones. These results provide a new model for understanding hydrologic-BGC controls over riparian floodplain function in the intermountain Western U.S.

Title: **Dynamic roots alter the legacy strength of terrestrial ecosystems in an Earth System Model**

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Project Lead Principal Investigator (PI): Max Berkelhammer

BER Program: ESS

Project: University project

Project Abstract:

The response of terrestrial ecosystems to climate perturbations typically persist longer than the timescale of the forcing, a phenomenon that is broadly referred to as *ecosystem legacy*. Understanding the strength of legacy is critical for predicting ecosystem sensitivity to climate extremes and the extent to which disturbances in land surface-atmosphere exchange might feedback onto the climate, for example, extending drought. Here we focus on the relatively unexplored role that changes in root profiles in response to perturbation (i.e. drought and pluvials) play in altering an ecosystem's recovery time. We use a series of global Earth System Model simulations with the E3SM model that include a dynamic root module where vegetation can forage for water and nutrients by altering their root profiles. As expected, the simulations show that in response to stress events most ecosystems deepen their root profiles. In semi-arid ecosystems, the deeper root profiles lead to a more rapid recovery (i.e. less legacy) than simulations without dynamics roots because access to deeper water pools after the initial event remains favorable. In wetter ecosystems, the development of deeper root profiles slows down the recovery timescale because water stress does not persist and the deeper root profile reduces access to nutrients in the shallower soils (i.e. more legacy). Similarly, in hyperarid systems the recovery is also delayed by deep root foraging due to reduced access to shallow soil water from smaller rain events. The results show that the response of root profiles to external forcing alters the legacy timescale in a direction that is predictable based on the baseline water stress. This dynamic is a critical component of global patterns of legacy that is not typically represented in Earth System Models. We will extend this global analysis to more detailed site scale studies as well as add more complex consideration of root allocation and turnover time schemes for fine root carbon with the E3SM model.

Title: **Water sources and resource limitations vary for trees along a hillslope transect in the East River Watershed**

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BER Program: ESS

Project: University project

Project Abstract:

In mountainous headwaters, there is substantial heterogeneity in physical drivers (e.g., soil moisture, depth to groundwater, snowpack and radiation) along hillslope transects that result in strong gradients in ecological properties, species distributions, and plant density. This coupled ecological and physical variability makes it difficult to develop integrated watershed-scale estimates of water (ET) and carbon fluxes using small fetch measurement approaches like eddy covariance. While remote sensing and physical models can provide spatially continuous information, these approaches require temporal and spatial networks of ground-based measurements for validation. Here, we report continuous (since 2019) sap flow measurements distributed across seven sites and three dominant species (aspen, fir and spruce) along a ~500 m elevational gradient in the East River Watershed. We used LiDAR estimates of tree height and density to generate half hourly stand-scale estimates of transpiration for these seven sites. A principal finding of this work is that transpiration near the toe slope converged on a value similar to estimates of energy-limited evapotranspiration from a nearby eddy covariance site situated in the riparian zone. This result suggests that transpiration accounted for almost all of evapotranspiration and that transpiration was not water limited. Moving up the hillslope, transpiration declined by almost an order of magnitude, reflecting both more water limitation as the vadose zone becomes more decoupled from groundwater and a relative increase in evaporation relative to transpiration as tree density declines. The exception to this elevation gradient was found in a convergence zone midway up the hillslope where transpiration reflected the energy-limited values seen at the toe slope and in the riparian zone. This spatial pattern also manifested following a major rainstorm: the energy-limited sites saw declines in transpiration (associated with reduced radiation) while the water-limited sites showed an increase in transpiration associated with the increase in soil moisture. Lastly, we used water isotope measurements of xylem water across the sites to show that the energy-limited sites drew more

heavily on winter precipitation through the summer, indicating their reliance on older water sources whose access does not vary a great deal seasonally, interannually or between species.

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

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BER Program: TES

Project: EPSCOR; University Award

Nitrogen (N) deposition has enhanced C storage in temperate forest soils. However, it remains unclear whether this soil C will persist as N deposition declines across the region. At the heart of this knowledge gap is the failure to link N-induced shifts in microbial biodiversity with traits that control microbes' ability to breakdown, assimilate or stabilize soil C. Given that this uncertainty directly impedes the ability of predictive models to project future soil C stocks, there is a critical need to determine how N-induced shifts in key microbial traits drive soil C stabilization. To address this uncertainty, our objectives are to 1) Quantify variations in taxon-specific and community-level microbial traits across gradients in microbial community composition, the distribution of ectomycorrhizal (ECM) and arbuscular mycorrhizal (AM) trees, and N availability and 2) Integrate these data into a novel predictive framework that enhances our ability to project the regional soil C consequences of N deposition in temperate forests.

We used quantitative stable isotope probing, metabolomics, and biogeochemical approaches to quantify microbial traits and their impacts on soil C cycling across scales. Under ambient N deposition, we show that soil microbes in AM soils have greater flexibility in their decomposition pathways than those in ECM soils. In AM but not ECM soils, the identity of the soil microbes decomposing litter as well as the resulting metabolites varied as a function of litter quality. Under elevated N, microbial diversity declined for both mycorrhizal types, but there were mycorrhizal-dependent shifts in diversity of taxa using aspartic acid. N fertilization led to diversity declines in AM soil microbes using the C and N from the amino acid. By contrast, ECM soil microbes only showed a decline for N. For both mycorrhizal types, however, our results suggest that there are mycorrhizal-dependent, decomposition pathways that respond differently to elevated N. We used these results to develop new microbial groups that classify microbes based on substrate preference in our plant-microbial interactions model, FUN-CORPSE. When confronted with data from laboratory and field measurements, the refined model was able to capture shifts in decomposition and the mineral stabilization of N. Coupled together, our experimental and model results highlight the importance of integrating state-of-the-art data on microbial traits and function into models to improve predictions of temperate forest responses to global change.

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

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Project Lead Principal Investigator (PI): Mariah Carbone

BER Program: ESS

Project: University Project

Project Website: None

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

Sticky Roots--Implications of Altered Rhizodeposition (Caused by Viral Infection) for Soil Carbon Processing in the Rhizosphere

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BER Program: ESS

Project: University project

Project Abstract: Mineral-associated organic matter (MAOM) is a dominant component of total soil carbon that can be protected from decomposition for millennia. We are studying diverse mechanisms by which plant roots can dislodge organic matter (OM) from soil minerals, enabling its mineralization by microbes and potentially moving associated nutrients into actively cycling pools. The importance of MAOM dynamics has spurred its inclusion in DOE's ELM model, but currently without addition of the root influence on stability of MAOM.

In ESS project (DE-SC0021093), we are using a novel tool to perturb belowground root-microbe-mineral interactions: viral infection. Infection decreases root:shoot ratio, so shoot nutrient demand must be met by more intensive mining of soil per unit root. Further, phloem flow is increased by infection, and roots become "sticky", suggesting altered amounts and/or types of rhizodeposits in the rhizosphere. Using this tool, to date we have experimented with a simple one virus (Barley Yellow Dwarf Virus)–one plant (*Avena sativa*) system. In soil, infected plants exhibited reduced photosynthesis and plant biomass, and root:shoot ratio. Phloem contents of leaves sampled using aphid stylectomy and analyzed by GC-MS included sugars, organic acids, and amino acids. In batch experiments, ^{13}C-labeled MAOM sorbed to lab-synthesized minerals was mobilized by a suite of common root-derived and microbial metabolites (oxalic acid, glucose, and catechol), via distinct direct rapid (mineral dissolution) and indirect slower (microbial) mechanisms. Analysis by FTICR-MS of liquid gathered from around roots of infected and uninfected plants grown hydroponically (therefore with no water or nutrient limitations) suggested a shift toward amino sugars and carbohydrates with infection. Natural perturbations of belowground function (such as via viral infection of plants) will inform incorporation and sensitivity testing of vulnerability of MAOM to rhizodeposition within ELM, potentially with notable implications for long-term soil carbon storage and nutrient availability.

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

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BER Program: SBR

Project: University Award

Project Abstract:

Biogeochemical cycling in subsurface aquatic systems is driven by anaerobic microbial processes that employ metalloenzymes. Pure culture studies reveal that low availability of trace metals may inhibit methanogenesis, mercury methylation, and reduction of N_2O to N_2 during denitrification. However, whether such limitations occur in natural subsurface aquatic systems is currently unclear. This project seeks to establish mechanistic links between trace metal availability and biogeochemical transformations in subsurface systems. Integrated field and laboratory studies of trace metal availability and biogeochemical processes are underway at riparian wetlands in the Tims Branch watershed at the Savannah River Site, marsh wetlands at Argonne National Laboratory, and the streambed of East Fork Poplar Creek at Oak Ridge National Laboratory. The speciation of trace metals in wetland soils and stream sediments shows surprising consistency across the field sites. Dissolved metals also show consistent uptake behavior by the soils and sediments but form distinct species at each site. Geochemical controls on trace metal availability may thus be site-specific despite similar native solid-phase speciation and binding affinities. Diffusive gradients in thin films (DGT) probes identify maximum porewater concentrations in stream sediment of ~10 nM for Cu and ~40 nM for Ni and Co, suggesting that these systems display metal-limitations. N_2O reduction is stimulated by Cu addition to stream sediments and riparian wetland soils, but marsh wetland soils display no N_2O accumulation even at background levels of Cu availability, i.e., no Cu limitations were apparent. Riparian and marsh wetland soils show little to no enhancement in CH_4 production in response to increases in dissolved Ni concentrations. Redox fluctuation experiments demonstrate that anoxic conditions promote Ni and Co availability and inhibit Cu availability in riparian wetland soils. Similar metal availability trends were displayed by stream sediments during redox fluctuations except for Ni, which showed greater availability under oxic conditions. Ongoing studies continue to explore metal limitations on CH_4 production and how formation of FeS in wetland soils and stream sediments affects metal availability.

Quantifying Microbial Roles in Environmental Iron Oxidation Via an Integrated Kinetics, ‘Omics and Metabolic Modeling Study

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Project Lead Principal Investigator (PI): Clara Chan

BER Program: ESS

Project: University project

Project Abstract:

Iron oxyhydroxides are extremely reactive environmental components and thus strongly influence biogeochemical cycles. Microorganisms catalyze iron oxidation to form iron minerals, but it is unknown how much environmental iron oxidation is biologically-mediated. We aim to quantify microbial iron oxidation rates and gain insight into the controls, toward an ultimate goal of integrating biotic iron oxidation into reactive transport models. Our work focuses on the Savannah River Site (SRS) in South Carolina. At Tims Branch, part of the Argonne National Laboratory Wetland Hydrobiogeochemistry SFA, where groundwater discharges into the stream, extensive iron-oxidizing microbial mats form and appear to be a major sink of uranium. Pond B, part of the Lawrence Livermore National Laboratory BioGeoChemistry of Actinides SFA, is an actinide-impacted seasonally-stratified pond with iron oxidation at the chemocline, which may be due to Fe-oxidizers.

Our approach combines field work, kinetics experiments, and metagenomics/metatranscriptomics coupled to metabolic modeling. Our objectives are to:

1. **Quantify biotic iron oxidation rates** in the field and in iron microbial mat incubations. We will compare these rates to abiotic rates to determine the relative contributions of microbes.
2. **Identify and quantify dominant iron-oxidizing microorganisms** and flanking community members at both SRS sites using genome-resolved metagenomics and metatranscriptomics and integrate the results to identify trophic status and carbon utilization of dominant iron oxidizers.
3. **Construct metabolic models of a well-studied iron-oxidizer and the most abundant and active iron-oxidizers and flanking organisms** to establish linkages between microbial Fe oxidation and C cycling.

The collaborations between UD, Argonne and LLNL SFAs, and the University of Minnesota-led project allow us to take advantage of field operations and hydrogeochemical observations from the locations that we plan to sample. Initial fieldwork (May 2021) included site scouting and sample collection for Objectives 1 and 2. A major project outcome will be iron oxidation rates and better protocols for obtaining reliable, replicable biotic iron oxidation rates for use in modeling, and an understanding of controls on iron oxidation. Our initial kinetics experiments on SRS mats have yielded promising results.

We will be generating a new library of Fe-oxidizer genomes from both SRS sites, and with transcriptomic results, we will characterize the trophic status of major Fe-oxidizers and ecological linkages that connect Fe and C cycling. This work sets the stage for our longer-term goal to link iron-oxidizer metabolic models and kinetics to biogeochemical/hydrological models to predict Fe, C, nutrient and contaminant metal cycling effects.

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

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Project Lead/Principal Investigator J. Coleman (UNCG), C. Trettin (USFS), A. Chow (Clemson)

BER Program: ESS
Project: University project

Mercury (Hg) is considered a global pollutant due to its long-range atmospheric transport and bioaccumulation in food webs. Forest ecosystems are thought to be sinks for Hg deposition through foliar uptake of dry elemental Hg(0). Hg can be transformed into a severe toxin when it can be converted to methylmercury (MeHg) when leaves are decomposed by the soil microbiome under anoxic conditions.

Efforts are underway in the southeastern US to convert as much as $2x10^6$ ha of stands of loblolly pine (*Pinus taeda*) to native longleaf pine (*Pinus palustris*). Intensive silvicultural practices will be used to facilitate conversion of the ecosystems. Those practices are known to temporarily alter the water balance of a site, but the effect of different silvicultural practices on Hg cycling and methylation in Southern pine watersheds is not well understood.

The aim of this two-year exploratory project is to characterize the influence of silvicultural practices on Hg cycling, especially Hg methylation. The work is being conducted within a first-order experimental watershed in on the Santee Experimental Forest in South Carolina. Tree harvesting (clear cutting) and thinning have been recently completed. We installed field transects from upland, riparian, to wetland with in-situ field sensors covering three portions of the experimental watershed - untreated (control), partial cutting (thinning), and complete tree removal (harvest). In addition to high frequency sampling of redox, water table depth, and soil temperature, we will conduct regular soil sampling along these transects through at least one year in order to characterize the changes of soil organic matter, total Hg (THg), and MeHg. We will also be sampling stream water and aquatic insects to characterize the movement of nutrients (i.e., C and N), THg and MeHg in the ecosystem.

The results should lead to the: 1) identification of biogeochemical "hotspots" of Hg methylation within Southern pine forest watersheds 2) relationships of silvicultural practices to MeHg production and accumulation in the food web; and 3) characteristics of organic matter that may be linked to the production of MeHg. The results, obtained by taking advantage of an experimental conversion of loblolly pine to a longleaf pine ecosystem, should be transferrable to understanding Hg biogeochemistry in other watersheds. Such an understanding may be useful in guiding forest managers on silvicultural practices that can mitigate or lessen Hg pollution. The findings from this study should also be useful in testing biogeochemical modelling of Hg dynamics.

Title: **Soil Carbon Cycling and Root Dynamics across Rainfall and Soil Fertility Gradients and with Drying in Lowland Tropical Forests of Panama**

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BER Program: ESS

Project: Early Career project

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

Project Abstract (400word):

Humid tropical forests contain some of the largest soil organic carbon (SOC) stocks on Earth. Much of this SOC occurs at depth in the soil profile, but controls over SOC storage and depth distributions, such as root turnover, climate, and soil properties, remain poorly understood. To address this, we measured SOC storage, soil C losses via respiration, fine root dynamics, soil nutrients, and aboveground characteristics across rainfall and soil fertility gradients on the Isthmus of Panama. We hypothesized that infertile soils have greater allocation of plant C to fine root biomass relative to fertile soils, and this corresponds to larger soil C stocks in infertile soils because of greater root biomass inputs. We also hypothesized that fine root biomass and soil C stocks are less vulnerable to drying in infertile soils relative to fertile soils, because of more conservative root growth strategies. We used 50 1-ha plots in distinct forests on different geological substrates for landscape-scale assessments, and we used four of these sites for a drying experiment. All sites are adjacent to long-term forest monitoring plots maintained by the Smithsonian Tropical Research Institute. The drying experiment was established in 2018, and uses ~50% throughfall diversion structures of clear roofing over 10x10m plots to divert throughfall out past 50cm-deep plastic-lined trenches (n=4).

We found that root biomass was the strongest predictor of soil C stocks to 1m depths, with additional predictive power provided by soil clay content, rainfall, and extractable base cations. We also found that the depth distributions of fine roots were inversely related to depth distributions of SOC. That is, infertile soils had relatively large stocks of root biomass in surface soils (0-20cm),

and large subsoil C stocks (40-100cm). Soil respiration varied greatly with season across the rainfall gradient. The magnitude of increased respiration during the wet versus dry season was correlated with soil available resin phosphorus, extractable base cations, and soil moisture variation. In the drying experiment, throughfall exclusion suppressed soil respiration during the transition from the dry to wet season, and suppressed surface fine root growth (0-20cm), similar to suppressed surface fine root growth during the dry season. These results suggest that global change effects on surface root growth in tropical forests might have cascading effects on subsurface SOC storage, affecting the large stocks of SOC contained in tropical forests. More research is needed to characterize the subsoil properties driving deep SOC storage in tropical soils.

Title: **Simulating Snow Patterns and Evolution in the East River SFA with a Distributed Snow Dynamics Model**

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

BER Program: SBR

Project: University project

Project Abstract:

Spatial and temporal patterns of snow accumulation and melt exert a dominant control on hydrologic and biogeochemical flows in temperate mountain catchments. Mountain snowpack states, fluxes, and properties exhibit extreme and scale-dependent variability, complicating efficient sampling and modeling. Capabilities for evaluating the impacts of system perturbations (e.g. climate shifts, radiative forcing by impurities, forest cover change) on system water availability and nutrient cycling are contingent on robust observations and simulations of seasonal snow dynamics at appropriate scales of action.
To explore snow accumulation and melt process dynamics over the meter to watershed scales, we have implemented a physically-based snow cover evolution model (SnowModel; Liston et al., 2006) at multiple grid resolutions, using different combinations of accumulation process sub-models. We first tested the model in Senator Beck Basin, a well-instrumented study site in southwest Colorado, and adjusted wind transport parametrization the main processes influencing snow pattern distributions in mountain head catchment. The sensitivity analysis of grid resolution and wind transport showed impacts on water available for runoff at the basin scale. Higher resolution and wind transport produce slower melt with delays of 10 days for 10 m to 100 m resolution and 48 days for without wind transport, due to snow drifts that last late into summer in the simulations with wind transport.

Model wind transport parameterization obtained in Senator Beck Basin were then transferred to the East River SFA where instrumentation is less-reliable. To improve model results and system disturbances impacts analysis, we have: (i) implemented and validated the albedo decay parametrization from Deems et al., 2013. and (ii) analyzed the forest impact on wind transport and redefine a new forest type to allow for forest sheltering of adjacent areas. The simulations over a recent set of years spanning high and low peak accumulation values, were forced with data assimilation model (HRRR) output, and are compared with ground measurements as well as

snow depth and snow water equivalent (SWE) maps from Airborne Snow Observatory flights. These results help characterize the snow hydrologic system in the East River and quantify the importance of snow distribution due to wind and gravitations transport at the watershed scale, setting the stage for future snow data assimilation work and for integration with simulations of connected systems within the SFA.

References:

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

Deems, J. S., T. H. Painter, J. J. Barsugli, J. Belnap, and B. Udall. 2013. Combined impacts of current and future dust deposition and regional warming on Colorado River Basin snow dynamics and hydrology. Hydrology and Earth System Sciences 17(11): 4,401-4,413. doi:10.5194/hess-17-4401-2013.

Title: **Use of Sequential Extraction and Mercury Stable Isotope Analysis to Assess Remobilization of Sediment-Bound Legacy Mercury**

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

Project Abstract:

Historical and ongoing releases of mercury (Hg) have resulted in a legacy of Hg contamination in streambed sediment, streambanks, and floodplain soils downstream of the Y-12 National Security Complex (Y12), along the flow path of East Fork Poplar Creek (EFPC) near Oak Ridge, Tennessee. Much of this legacy Hg resides in relatively insoluble fractions, and has thus been considered to have little impact on dissolved Hg concentrations. However, recent studies suggest that dissolved Hg from hyporheic pore water contributes as much as a third of downstream dissolved Hg loads during base flow conditions. The goal of this project was to assess how anthropogenic legacy Hg is remobilized from streambed sediment to stream water. We used sequential extractions to quantify the different forms of Hg in the sediment, and Hg stable isotope analysis to track the cycling of Hg among those pools. Mercury isotope analysis of bulk streambed sediment revealed patterns that are consistent with equilibrium isotope effects between coexisting Hg(0) and Hg(II), which likely overprinted isotopic signatures imparted by kinetic Hg oxidation and reduction reactions, a phenomenon that had previously been demonstrated in laboratory experiments but not identified *in situ.* Mercury isotopic analysis of the five-step sequential extractions revealed that weakly-bound and recalcitrant Hg pools in the sediment were isotopically similar to one another, suggesting that the weakly-bound pools were derived from the recalcitrant pools by dissolution and rapid re-adsorption. This weakly-bound Hg can then be remobilized to the hyporheic pore water and surface water as dissolved Hg. Organically-bound Hg pools in the sediment were isotopically distinct at upstream sites, but converged with the isotopic composition of weakly-bound and recalcitrant sediment Hg pools along the flow path (shifting toward higher δ^{202}Hg and lower Δ^{199}Hg values). A similar trend in the mercury isotopic composition of suspended particulates and streambed biofilm has been previously observed. This suggests both physical mixing among these components and the transfer of weakly-bound sediment Hg into biofilm and suspended particulates which are then reincorporated into the organically-bound sediment Hg pool. Overall, these sediment sequential extractions and Hg isotope analyses provide evidence that sediment-bound legacy Hg within the streambed can be remobilized. Thus, large pools of recalcitrant legacy Hg have the potential to be a long-term source of dissolved Hg to stream water as well as a source of Hg to streambed biofilm, a basal resource of aquatic food webs.

Title: *Deciphering controls on metal migration within floodplains: The critical role of redox environments on metal-organic complexes*

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Project Lead Principal Investigator (PI): Scott Fendorf

BER Program: ESS

Project: University Project

Project Abstract:

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 remains largely unexplored, although it may be a primary determinant of dissolved metal concentrations and migration.

The overarching goal of our project is to determine the effect of redox conditions resulting from differing hydrologic regimes on formation and transport of soluble metal-organic complexes. To meet our research goal, we are using a combination of field measurements and laboratory experiments to examine the relationships between redox conditions, functionality of dissolved organic matter, and metal speciation (specifically examining metal-ligand complexes). Continuous monitoring of floodplain biogeochemical conditions through climatic extremes at East River provide a unique look at metal-OM complexes. We have developed novel methods to separate, quantify, and characterize organic-metal complexes in natural DOM that pair with field experiments comprising floodplains having systematic variation in biogeochemical conditions. We evaluated the role of column chemistry and solvent composition on separation and recovery of complexes of metals ranging in binding preferences (Al, Fe, Co, Ni, Cu, Zn, Cd, Pb) with NOM. We are also developing a comprehensive computational approach for molecular characterization of metal-organic species, which merges LC-coupled high resolution (HR) mass spectrometry and ICP-MS analysis. We are employing these methods to characterize metal-organic species in soils from the East River and Savannah River watersheds. Our findings illustrate changes in binding preference of DOM from differing redox environments for Cd and Ni, metals having contrasting ligand preferences. Specific ligand selectivity and exchange changes depending on the environmental biogeochemical conditions. Our work is advancing a process-based understanding

of metal fate and transport within watersheds, focusing principally on the dynamic hydrologic states of floodplains. Ultimately, our work is helping to advancing a robust predictive understanding of how hydrologic changes in watersheds affect water quality and inorganic element/contaminant loading.

Peatland hydrology across scales: seasonal and interannual controls of water table and carbon emissions

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BER Program: TES

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

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

To date, we have demonstrated the strong influence of water table elevations on the temperature sensitivity of CH_4 emissions, using a newly developed eddy covariance dataset spanning eleven years at MEF (Feng et al. 2020). Specifically, higher water tables dampen the springtime increases in CH_4 emissions as well as their subsequent decreases during the fall, resulting in hysteresis. These results imply that any hydroclimatological changes in peatlands that shift seasonal water availability from winter to summer will increase annual CH_4 emissions, even if temperature remains unchanged. To further investigate seasonal hydrological changes, we installed automated water table gauges across four bog-forest boundaries (the “lagg”) in two watersheds at MEF, which are hotspots of intense biogeochemical activity. These measurements will give us new information about the extent of lagg expansion and contraction during high intensity rainfall and snowmelt events. Finally, the hydrological connectivity between upland forests and low-lying bogs are investigated during the snowmelt period using existing data for snow and frost depth, water table elevations, and streamflow. Preliminary results show decrease in water table elevation and annual streamflow despite an increase in precipitation, due to the dominant role of evaporative demand that decrease surface water storage in snowpack and bogs.

References:

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

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

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BER Program: Environmental System Science

Project: University Project

Project Website: N/A

Project Abstract: The timing, rate, and spatial extent of deliver of water to the critical zone in mountain regions is exerts a fundamental control on biogeochemical processes but is itself a complex process that involves interactions between the atmosphere, vegetation, topography, and subsurface. In particular, water delivery to the critical zone is fundamentally constrained by the quality (timing, magnitude, and phase) of the available precipitation data, which is often limited in high elevation mountain watersheds. We implement a 30-year long regional climate reconstruction using the Weather Research and Forecasting model, run at convection-permitting resolutions, covering the East River and Upper Colorado river basin. To validate the simulated precipitation fields, we leverage snow remote sensing, station meteorological measurements, streamflow records, and parsimonious water balance models within Bayesian data-fusion and inference methodology to create confidence intervals on annual, watershed scale precipitation. Through this effort we are able to synthesize precipitation datasets at higher spatiotemporal resolution, greater accuracy, and better characterized uncertainty than other precipitation products. To enhance constraints on the spatiotemporal variability of snow cover in the East River watershed, we simultaneously synthesized a long-term, high spatiotemporal resolution dataset of snow-covered area (SCA) through satellite data fusion. Specifically, we applied the Spatial and Temporal Adaptive Reflectance Fusion Model (STARFM) to create a 30 m, daily resolution dataset for an approximately 20 year long period, allowing us to examine patterns of seasonal snow cover. This novel application of STARFM for snow cover estimation combines low spatial and high temporal resolution data from MODIS (500-m, daily) with high spatial and low temporal resolution data from Landsat (30-m, 16 days). As an example application of this dataset, we examine percent annual snow cover in the East River for a wet, dry, and average water year. We find that predictable patterns of SCA occur over those years, with the highest percent annual snow cover occurring during the wet year and the lowest occurring during the dry year. Despite these differences, however, elevation is clearly the dominating factor in determining the spatial variability of snow cover in the landscape for all three water years. These

datasets are being made available to the Watershed Function and broader science communities to better constrain estimates of the rate of delivery of water to the critical zone through integrated hydrological modeling efforts, and to supplement gaps in observational data products. Some relevant examples of how these data are used are provided.

Metagenomic characterization of subsurface Thaumarchaeota populations in hydrologically-variable floodplain sediments

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BER Program: ESS
Project: University project DE-SC0019119

The terrestrial subsurface microbiome contains vastly underexplored phylogenetic diversity and metabolic novelty, with critical implications for global biogeochemical cycling. Among key microbial inhabitants of subsurface soils and sediments are Thaumarchaeota, an archaeal phylum encompassing the ammonia-oxidizing archaea (AOA). Although AOA have been studied extensively in topsoils, our understanding of the diversity, ecophysiology, and activity of these critically important nitrogen-cycling organisms in deeper soils/sediments is limited. Our recent analysis of subsurface microbial communities (based on both 16S rRNA and *amoA* ammonia monooxygenase genes) within hydrologically-variable floodplain sediments in the Wind River Basin near Riverton, WY revealed that AOA were the predominant ammonia-oxidizers and that their community structure shifted dramatically with depth. In order to understand the ecophysiological adaptations of these subsurface AOA, we used genome-resolved metagenomics to examine Thaumarchaeota populations spanning 11 distinct depths along a 234 cm depth profile at Riverton site KB1. Phylogenomic analysis of metagenome-assembled genomes (MAGs) indicated a pronounced shift in AOA populations: in the well-drained top ~100 cm of the profile, the 'terrestrial' Nitrososphaerales lineage was dominant; whereas in deeper, moister, oligotrophic sediment layers, members of the typically 'marine' Nitrosopumilales lineage were most pervasive. This vertical zonation in thaumarchaeal population structure was similarly evident in the relative abundances of lineages, estimated based on read mapping against MAGs. Our results suggest that hydrological variables, particularly proximity to the water table, impart a strong control on the ecophysiology of Thaumarchaeota in alluvial sediments. To complement our detailed spatial (vertical) characterization of AOA communities at site KB1, we recently investigated subsurface microbial community composition over both time and space (depth) at a nearby Riverton site (Pit2) through a full seasonal hydrologic cycle of water table rise, flooding, and summer drought. In particular, we obtained 16S rRNA gene amplicon data from samples collected monthly (April to September 2017) from 7 distinct subsurface layers [topsoil, evaporite, sand, evaporite/clay, transiently-reduced zone (TRZ), clay, and aquifer], allowing spatiotemporal AOA dynamics to be examined within the context of the overall microbial communities and a suite of hydrogeochemical measurements. We also selected 40 of these Pit2 samples for metagenomic sequencing, which has resulted in the generation of >3000 high-quality MAGs, many of which correspond to diverse AOA as well as nitrite-oxidizing bacteria. Overall, this study is yielding unprecedented genomic and ecophysiological insights into the microbial communities responsible for nitrification in subsurface floodplain sediments directly influenced by hydrological fluctuations.

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

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

Project Abstract:

Rapid warming in the Arctic is driving changes in the structure and composition of tundra vegetation communities. These changes are expected to alter key biogeochemical and physical processes that feedback to climate. However, the magnitude of this feedback is highly uncertain due to limited understanding of spatial variation in plant functional traits and the over-simplification of traits in current Earth system models. To facilitate improved representation of aboveground and belowground traits in models, we will characterize directly observable plant functional traits from remotely sensed data, and predict non-observable (e.g., belowground) traits by leveraging trait-environment relationships and trait covariation. Additionally, we will integrate trait information into the Terrestrial Ecosystem Model (TEM) to quantify and predict regional C balance in the Alaskan tundra. We will test four hypotheses: (1) Plant functional traits are predominantly shaped by climate, with local soil moisture and active layer depth moderating trait response to climate, but optimal trait values for a given environment depend on community type because plant functional types (PFTs) have different sensitivities to altered resources associated with climate warming. (2) Trait dispersion depends on environmental stress; where environmental conditions are more favorable for growth, there is greater variation in traits and greater trait diversity; (3) Root traits are predictable from leaf and size traits, climate and soil factors; and (4) Variation in traits affect Arctic C balance. Leaf traits as they relate to photosynthetic parameters will have the strongest effects on C uptake. Root traits will exhibit fewer direct effects on C uptake but will be important in supporting nutrient uptake that then influences C uptake. To test these hypotheses, we will study the variation in plant traits across the major tundra vegetation communities present along local soil gradients nested within a macroclimate gradient in northern Alaska, quantifying trait-environment relationships and trait covariation at the community- and PFT-levels. Using machine-learning approaches, we will integrate ground-based measurements with information derived from multi-scale remote sensing platforms from drone, hypertemporal, LiDAR, and hyperspectral imagery to produce maps of leaf, size and root traits, greatly expanding the trait information available for modelers. We will use Bayesian data-model fusion methods to improve the parameterization and formulation of TEM, which is widely used in Arctic carbon studies, and perform simulation experiments to evaluate how differences in plant functional traits affect C dynamics.

Particulate organic matter (POM) transport and transformation at the terrestrial-aquatic interface

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This project examines the input and metabolism of particulate organic matter (POM) in near-surface riverbed sediments at the PNNL SFA Hanford 300 Area study site, where large fluctuations in water stage drive periodic fluid flow into or out of the hyporheic zone. Such POM input has the potential to strongly impact the biogeochemistry of both the river itself as well as the hyporheic zone (or, more broadly, the hyporheic corridor) that is connected hydrologically to the river. The central hypothesis of our project is **that advective introduction of POM into permeable riverbed sediments will result in its accumulation to levels much higher than the input concentration, which in turn will drive relatively rapid rates of microbial carbon and nutrient (N) metabolism. Additionally, we hypothesize that POM degradation may result in the export DOC and/or inorganic nitrogen into the underlying hyporheic zone.**

Current research efforts are examining in situ POM deposition and its potential degradation in the Columbia Riverbed using custom designed "POM traps" and in situ DO measurements to develop a qualitative model of POM and DO consumption in riverbed sediments to inform our laboratory mesocosm and column experiments. Smaller-scale, horizontal column experiments using Hanford Formation sand, sieved to remove fines, and POM, grown from a Columbia River inoculum, reveal that POM is primarily removed through filtration and a large portion of the POM is remobilized upon flow reversal. This data has been used to develop a quantitative model describing POM immobilization and remobilization. Larger-scale vertical column experiments, using ashed Columbia Riverbed sediment, have revealed that at high POM densities, both settling and advective transport are critical factors in vertical POM movement, with filtration also being the primary POM retention mechanism. This research directly addresses priority research objectives related to the need to quantify and predict how hydrology drives fine-scale biogeochemical processes in surface-subsurface systems, as well as quantifying how biological, abiotic-biotic interactions and molecular transformations control the mobility of nutrients and critical biogeochemical elements.

Hydrometeorological sensitivities of net ecosystem carbon dioxide and methane exchange of an Amazonian palm swamp peatland

Tim Griffis[1*], Tyler Roman[2], Fenghui Yuan[1], Jeff Wood[3], Julian Deventer[1,4], Lizardo Fachin[5], Jon Rengifo[5], Dennis Del Castillo[5], Erik Lilleskov[6], Randy Kolka[2], Rod Chimner[7], Craig Wayson[8], Kristell Hergoualc'h[9], John Baker[10], Hinsby Cadillo-Quiroz[11] and Dan Ricciuto[12]

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Project: University Project Award Number DE-SC0020167
Project Website: https://biometeorology.umn.edu/research

Project Abstract:
Tropical peatlands are a major, but understudied, biophysical feedback factor on the atmospheric greenhouse effect. The largest expanses of tropical peatlands are located in lowland areas of Southeast Asia and the Amazon basin. The Loreto Region of Amazonian Peru contains ~63,000 km^2 of peatlands. However, little is known about the biogeochemistry of these peatlands, and in particular, the cycling of carbon dioxide (CO_2) and methane (CH_4), and their responses to hydrometeorological forcings. To address these knowledge gaps, we established an eddy covariance (EC) flux tower in a natural palm (*Mauritia flexuosa* L.f.) swamp peatland near Iquitos, Peru. Here, we report ecosystem-scale CO_2 and CH_4 flux observations for this Amazonian palm swamp peatland over a two-year period in relation to hydrometeorological forcings. Seasonal and short-term variations in hydrometeorological forcing had a strong effect on CO_2 and CH_4 fluxes. High air temperature and vapor pressure deficit (VPD) exerted an important limitation on photosynthesis during the dry season, while latent heat flux appeared to be insensitive to these climate drivers. Evidence from light-response analyses and flux partitioning support that photosynthetic activity was downregulated during dry conditions, while ecosystem respiration (RE) was either inhibited or enhanced depending on water table position. The cumulative net ecosystem CO_2 exchange indicated that the peatland was a significant CO_2 sink ranging from −465 (−279 to −651) g C m^{-2} y^{-1} in 2018 to −462 (−277 to −647) g C m^{-2} y^{-1} in 2019. The forest was a CH_4 source of 22 (20 to 24) g C m^{-2} y^{-1}, similar in magnitude to other tropical peatlands and larger than boreal and arctic peatlands. These measurements have been used to help parameterize the Energy Exascale Earth System Model (E3SM) land surface component (ELM). Initial modeling results demonstrate that ELM can capture the seasonal and diel cycles of CO_2 and CH_4 fluxes. Further, we identified that the photosynthetic response at this tropical peatland site is very sensitive to air temperature, while CH_4 production is more sensitive to water condition, which can significantly influence its carbon budget. Ongoing model analyses are exploring potential biophysical feedback processes associated with changes in hydrometeorology for this region.

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

Erich Hester,[1*] W. Seth Lotts,[1] Hector Monterroso,[1] Kyle Strom,[1] and Mark Widdowson,[1]

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Project Lead Principal Investigator (PI): Erich Hester

BER Program: Environmental System Science

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

Project Abstract: The area beneath and adjacent to river channels where surface water and groundwater interact in shallow sediments is known as the hyporheic zone. The hyporheic zone is often more reactive than overlying surface water or deeper groundwater, and thus is an important area for chemical transformation and contaminant attenuation within river corridors and watersheds. This exploratory project is developing a predictive mechanistic modeling approach to quantify the effects of surface water fluctuations and bed migration on hyporheic zone microbial community distribution and hence hyporheic biogeochemical cycling. We started this work by focusing on 1) relatively low flows (e.g., baseflow and modest increases for hydropower peaking) across the annual cycle because they occur for most of the year and sediment migration is well understood, and 2) riverbed dunes which are widespread in larger streams and rivers and often dominate hyporheic effects on water quality, and 3) the effects of the interaction of oxygen and carbon infusion from surface water and sediment migration on microbial heterogeneity, aerobic metabolism, and denitrification. We are linking a series of existing models that simulate surface water hydrodynamics (OpenFOAM), groundwater flow (MODFLOW), and groundwater transport/reaction (SEAM3D). We are currently 1) developing and testing a moving frame of reference (MFOR) modeling approach to simulate dune migration effects on biogeochemical transformations through modification of SEAM3D, and 2) testing existing microbial population growth and decay functions of SEAM3D. After linking and testing are finished, we will conduct sensitivity analyses of controlling factors such as hydraulic, biogeochemical, and microbial model parameters and boundary conditions. Given the recent start to this project, results at the time of this writing are limited. But we anticipate quantifying the effect of varying the ratio of dissolved oxygen to dissolved organic carbon concentrations in surface water, surface water and groundwater boundary heads, bedform movement celerity, and sediment hydraulic conductivity on microbial biomass and distribution, microbial response time, and aerobic oxygen consumption and nitrate consumption due to denitrification in hyporheic zone sediment. These results will have important implications for material processing in watersheds where microbial and sediment dynamics are important.

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

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Project Lead Principal Investigator (PI): Caitlin Hicks Pries

BER Program: ESS

Project: University-led research

Project Website: NA

Project Abstract: Mycorrhizal fungi provide plants with nutrients in return for photosynthate, linking above and belowground processes. Forests dominated by arbuscular (AM) versus ectomycorrhizal (EcM) fungi differ in total soil carbon (C) and nitrogen (N) pools, but their effect on the distribution of C and N within mineral soils is uncertain. We measured the effects of mycorrhizal associations on the distribution of soil C and N among particulate and mineral fractions in four forests across the Eastern United States, which had gradients of EcM-associated tree basal area but differed in their dominant tree families. Within each plot, we used ITS sequencing to characterize communities of EcM fungi. We expected that the amount of C and N in mineral-associated pools would decrease as the basal area of EcM trees increased, but that pattern was only observed in half of our sites. We found that the EcM fungal communities and the dominant tree families were better predictors of mineral-associated C and N than the proportion of EcM-associated trees. Thus, not all EcM fungi have similar effects on soil biogeochemistry. We are currently investigating two hypothesized drivers for how soil C and N are affected by mycorrhizal associations: inherent differences in 1) litter quality and 2) nutrient acquisition strategies in a large scale in situ decomposition experiment with six different types of dual ^{13}C and ^{15}N-labeled litter. We have placed litter in soil mesocosms at forests in NH, IL, and GA where each have six plots differing in the abundance of EcM-associated trees and the family of the dominant EcM trees. Our initial results suggest that fungal communities are more important drivers of how soil carbon and nitrogen are stored than litter quality. We will explore the implications of these findings for soil carbon storage using a modified CORPSE model that takes into account differences in fungal community function.

Title: Whole Ecosystem Warming Stimulates Methane Production Fueled by Plant Metabolites in Peatlands.

Joel E. Kostka[1*], Rachel Wilson[2], Caitlin Petro[1], Tianze Song[1], Max Kolton[1], Eric Johnston[3], Christopher Schadt[3], Jeff Chanton[2] and Paul Hanson[3].
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Project Lead Principle Investigator (PI): Joel E. Kostka
BER Program: ESS
Project: University project
Project Website: Affiliated with SPRUCE; https://mnspruce.ornl.gov/
Project Abstract: Climatically sensitive, northern peatlands store approximately one-third of Earth's terrestrial soil organic carbon. The objective of this project is to quantify the response of belowground carbon stores, greenhouse gas emissions, and heterotrophic microbial communities in peatlands to environmental disturbance (warming, CO_2 enrichment). Our investigations leverage the Spruce and Peatland Responses Under Changing Environments(SPRUCE) experiment where air and peat warming are combined in a whole ecosystem warming approach. We hypothesized that, in addition to stimulating microbial activity directly, warming would enhance the production of plant-derived metabolites, resulting in increased labile organic matter inputs to the surface peat, thereby further enhancing microbial activity and greenhouse gas production. In support of this hypothesis, significant correlations were observed between metabolites and temperature consistent with increased availability of labile substrates which may stimulate more rapid turnover of microbial proteins[1]. Production of the potent greenhouse gas methane(CH_4) was shown to increase at a faster rate in comparison to carbon dioxide(CO_2) in response to warming. Predominant methanogens were identified and the dominant species were highly similar to a Ca. Methanoflorens stordalenmirensis genome recovered from a peatland in northern Sweden. While Methanoflorens is thought to produce CH_4 from hydrogen and CO_2, the organism remains uncultivated and our metagenome data suggest methane production from alternate metabolic pathways. Further, other methanogens were also detected that produce methane from methylated compounds such as methanol, and multiple lines of evidence (isotopes, metabolomes, metagenomes, tracer studies) point to a shift toward methylotrophic methanogenesis with warming. While our results clearly show that methanogens in SPRUCE peat are responding to warming, no significant change in the absolute abundance of methanogens, as determined by qPCR, has yet been detected. We thus interpret the observed responses as a more rapid, pronounced change in the physiology or activity of methanogens in response to temperature, whereas a change in abundance or biomass is likely more muted and difficult to detect beyond natural heterogeneity. Methanogens thus appear to increase their efficiency, resulting in an increase in the CH_4 to CO_2 ratio. While soil carbon has accumulated over millennia in peatlands, our results demonstrate that the vast deep carbon stores are

vulnerable to microbial decomposition in response to warming. Elevated rates of methanogenesis are fueled by plant metabolites, Thus, as peatland vegetation trends towards increasing vascular plant cover with warming, we can expect a concomitant shift towards increasingly methanogenic conditions,which are likely to persist resulting in amplified climate-peatland feedbacks.

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Hydrological and Biogeochemical response to warming in a high elevation mountain watershed in Colorado

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High-elevation mountain watersheds are undergoing rapid warming and declining snow fractions worldwide, causing earlier and quicker snowmelt. Understanding how this hydrologic shift affects subsurface flow paths, biogeochemical reactions, and solute export has been challenging due to the entanglement of hydrological and biogeochemical processes. This work aims to understand the impacts of shifting climate on water partitioning and stream chemistry in Coal Creek, a high-elevation catchment (2,700 – 3,700 m, 53 km^2) in Colorado. Coal Creek has experienced a higher rate or warming than surrounding low-laying areas [*Zhi et al.*, 2020]. This warming corresponds with dynamic and increased responses from biogenic solutes, whereas geogenic solute and dissolved inorganic carbon (DIC) behavior has remained relatively unchanged. DIC was analyzed along with DOC to incorporate both carbon component products of soil respiration (DOC & CO_2) while also representing chemistry consistent with shifting subsurface flow sources [*Zhi and Li*, 2020; *Zhi et al.*, 2019]. DOC has experienced the largest concentration increase (> 3x). Analysis of annual averages show flow-weighted concentrations are positively correlated with daily minimum air temperature. The contrasting behavior of DOC and DIC indicate climate change and warming are driving changes in organic matter decomposition and increasing concentrations of biogenic species produced in the shallow soil zone, whereas DIC and deep zone species are less affected by climatic changes and more by water partitioning. DOC and DIC data were used along with the reactive transport model BioRT-Flux-PIHM to quantify rates of organic matter decomposition, soil respiration, and subsurface flow path partitioning under different climate forcings at a watershed scale. Preliminary modeling results show that temperature is causing earlier snowmelt, earlier stream flow generation, and lower peak discharge. As stream flow generation occurs earlier so do DOC flushing and DIC dilution events. Additionally, following the post snowmelt times DOC concentrations show a greater increase under warming scenarios. These results indicate earlier melt is partitioning through the shallow zone and warming temperatures are driving increased DOC production. Most process-based studies lack a watershed scale understanding of carbon transformation and flow path alterations. This work shows complex hydrological and biogeochemical coupling at the watershed scale to illustrate how water flow paths and quality are responding to a changing climate in high-elevation mountain watersheds.

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Zhi, W., Williams, K.H., Carroll, R.W.H., Brown, W., Dong, W., Kerins, D. and Li, L. (2020), Significant stream chemistry response to temperature variations in a high-elevation mountain watershed, *Communications Earth & Environment*, 1(1), 43.

Title: **Mangrove ecosystems under stress: from carbon sink to source**

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

BER Program: ESS

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

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

Project Abstract: Mangroves grow along coastlines and intertidal zones, and are therefore very rarely limited by water availability. However, during the dry season, these ecosystems behave more similarly to semi-arid ecosystems than like well-watered forests. Mangroves likewise provide a critical carbon sink sequestering carbon at a rate disproportionate to ecosystem extents. However, these delicate systems are threatened by anthropogenic activity and changes in climate. This project supports mangrove monitoring in four sites across the globe: from humid (Panama) to arid (Abu Dhabi) and at the northern (Texas) and southern (Victoria, Australia) growth limits. At the northern and southern extents, mangrove range expansion is limited by freezing conditions. We show eddy covariance fluxes of carbon and water exchange in the newly constructed Port Aransas, Texas mangrove monitoring station during the prolonged hard freeze in February 2021. As a result of the freezing conditions, mangroves in the site lost >90% of their leaf area causing the ecosystem to rapidly shift from a carbon sink to a carbon source. Encouragingly, we see evidence of a fast recovery and the mangrove population re-sprouting from roots.

Modeling the water and carbon dynamics of mangrove forests is a critical task for developing robust models of coastal climate processes. Here, we present the initial development of a salt-tolerant water uptake model for the FETCH2 advanced vegetation hydrodynamics model that will be capable of mechanistically simulating osmoregulation by halophytes. FETCH2 approximates water flow through xylem as flow through porous media and accounts for dynamic changes to conductance and capacitance of plant tissues caused by changes in water content. Parameter sets within FETCH2 are based on measurable hydraulic traits. Studies have shown that many such traits can be highly plastic and vary spatiotemporally. Therefore, we leverage our extensive field study and a greenhouse based study of mangrove hydraulic traits and their variability. Our four field study sites are positioned to promote analysis of mangrove forest function across both humidity and salinity gradients which are predicted to change in response to disturbances such as sea level rise, precipitation variability, inundation frequency, and increased atmospheric CO_2. Within the greenhouse, we are able to test for species and population differences in adaptation and

acclimation of different hydraulic traits to fluctuating humidity and temperature environments. These data will ultimately be used to parameterize the FETCH2 halophyte model with the ultimate goal to integrate FETCH2 into DOE’s functionally assembled terrestrial simulator (FATES) within E3SM.

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

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Project Lead Principal Investigator (PI): David Medvigy

BER Program: ESS

Project: University project

Project Website: n/a

Project Abstract: Trees and lianas dominate the canopy of tropical forests and comprise the majority of tropical aboveground carbon storage. These growth forms respond differently to variation in climate and resource availability, and their responses to future climate change are poorly understood. The overarching objectives of this project are to carry out an observational campaign to advance our understanding of liana traits and strategies, develop a liana-enabled forest dynamics model that leverages our observations, and to engage with the Earth System Modeling (ESM) community to plan for the eventual inclusion of lianas into ESMs. Here, we report on four activities which have brought us closer to meeting these objectives. (1) We have constructed trait distributions for lianas and trees, and identified those traits which differed between lianas and trees. The most striking difference was found for sapwood-specific hydraulic conductivity, which was three times larger in lianas than trees. We 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. (2) We 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-meter-cubed voxels. Thus, for a given host tree canopy, our scheme specifies where it is that lianas prefer to grow new leaves. We have carried out a sensitivity analysis and variance decomposition with respect to model parameterization. (3) We are quantifying liana demography in two sets of plots in Guanacaste, Costa Rica. These plots were established between 2008-2016 and span successional and edaphic gradients. Some of the plots are being subjected to nutrient fertilization and/or throughfall exclusion. Current measurements include tree and liana diameter growth, death, and recruitment. Further, each year we record an index of liana load on each tree, using a 0-3 point ordinal scale. We are currently analyzing demographic rates as a function of liana load. (4) We are measuring litterfall and fine root production in the plots. We installed 30 cm deep root ingrowth cores in 18 plots in December 2020. We are further partitioning fine root production

into lianas versus trees using molecular analyses. We have begun preliminary tests to optimize the primers and PCR conditions for the molecular analyses.

Title: **Increased Plant-Mediate Oxygen Transport in Response to Elevated CO_2 But Not Warming in the Salt Marsh Accretion Response to Temperature eXperiment (SMARTX)**

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Project Lead Principal Investigator (PI): Pat Megonigal

BER Program: ESS

Project: SMARTX

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

Project Abstract:

Coastal wetlands are hotspots of carbon sequestration, cycling, and export that regulate the biogeochemistry of coastal rivers, estuaries, and continental shelves, but are poorly represented in Earth System Models. The Salt Marsh Accretion Response to Temperature eXperiment was established at the Global Change Research Wetland in 2016 to advance model representations of the complex interactions between plants, microbes, and hydrology in forecasts of coastal wetland responses to global climate change. We actively manipulate whole-ecosystem temperature and atmospheric CO_2 concentration through feedback-controlled heating from the plant canopy to 1.5 m soil depth and CO_2 addition (eCO_2).

Complexity in tidal wetland responses to global change arises from the fact that wetland plants simultaneously regulate supplies of electron donors (organic carbon) and electron acceptors (molecular oxygen). We found that warming and eCO_2 generally increase aboveground net primary productivity (NPP) but have more complex and non-linear effects on belowground NPP. These non-linear belowground plant responses are driving key soil biogeochemical processes such as redox potential, soil carbon sequestration, and methane emissions. A custom-designed automated redox system in a subset of the plots shows that eCO_2 increases redox potential by up to 150 mV, presumably by increasing O_2 transport through plant biomass. Warming dramatically

increases CH_4 emissions through increased labile carbon supply but warming crossed with *e*CO_2 caused CH_4 emissions to decline dramatically because of increased CH_4 oxidation. Plots with the highest belowground NPP tended to have the highest rates of soil carbon sequestration, except when warming was crossed with *e*CO_2, suggesting that increased plant O_2 transport has enhanced soil organic matter decomposition. FTCIR of porewater dissolved organic carbon indicates that *e*CO_2 may cause a loss of aromatic compounds, consistent with an increase in plant O_2 transport. Collectively, our results show that plant O_2 transport must be represented in numerical models to forecast key coastal wetland biogeochemical phenomena.

The Coastal Carbon Ecosystem Model (CCEM) is a point-based model with plant-sediment feedbacks to forecast changes in soil elevation and soil carbon stocks over decade to century timescales. We modified the CCEM to include semi-empirically derived relationships between belowground biomass and soil organic matter decomposition. Model results indicated that *e*CO_2 and SLR interact synergistically to increase soil carbon burial, but feedbacks between plant biomass and decomposition (priming by plant O_2 transport) reduced the impact of *e*CO_2 on soil carbon accumulation. Such feedbacks are being incorporated into the land component of the Energy Exascale Earth System Model.

Biogeochemical Consequences of the Hydrologic Connection Between Permafrost-Thaw Bogs and Surrounding Peat Plateaus: Advective Heat Transport in Permafrost Landscapes

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Project Lead Principal Investigator (PI): Rebecca B. Neumann
BER Program: TES
Project: University project

When ice-rich permafrost thaws, the ground subsides, creating thermokarst features such as thaw bogs. While this type of landscape transformation releases carbon stored in permafrost into the atmosphere, on longer time scales, it facilitates sequestration of atmospheric carbon in plant biomass because permafrost thaw releases plant-available nutrients and wetlands are highly productive. However, wetlands also generate methane, which is a potent greenhouse gas. Methane emissions from thermokarst bogs can cause these carbon-sequestering systems to have a positive global warming potential.

Data previously collected by the research team from a thaw bog in Interior Alaska demonstrated that rainfall early in the growing season notably increased CO_2 uptake and CH_4 emissions by the bog. Water from the surrounding permafrost-peat-plateau flowed through the peat soils and penetrated into the bog, rapidly warming bog soils down to deep depths (~80 cm). The warm, deep bog soils early in the growing season supported microbial and plant processes that enhanced CO_2 uptake and CH_4 emissions. Thaw bogs often represent topographically low points in the landscape, and thus they receive and collect runoff from the surrounding landscape. However, the hydrologic connection between bogs and the surrounding permafrost plateaus (the bog-watershed connection), and the ability of this connection to impact biogeochemical processes in the bog, is not traditionally recognized in field studies nor included in models.

Our project is advancing understanding of the bog-watershed connection, clarifying the conditions under which it results in the transport of thermal energy into bog and impacts land-atmosphere exchange of carbon. We are conducting fieldwork at a well-instrumented, thawing bog complex in Interior Alaska and performing Earth System modeling. Field data thus far indicate that bogs that receive proportionately more water from the surrounding watershed emit more methane. Through coupled modeling of lateral water and heat transport with Energy Exascale Earth System Model (E3SM) land model (ELMv1-ECA), we have confirmed the important role of advective heat transport in affecting bog soil temperatures and CH_4 emissions. Specifically, results show that incorporating lateral advective heat transport improved simulated soil-temperature and moisture profiles, active layer thickness, and bog area inundation dynamics along two simulation transects that extend from the peat-plateau to the bog, aligning with major sensor locations at the field site.

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

Title: Using root and soil traits to forecast woody encroachment dynamics in mesic grassland

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BER Program: ESS

Project: University Award

Project Abstract:

Grasslands are a widespread and globally important biome providing key ecosystem services including C storage and regulation of the water cycle. Grasslands face multiple threats, including increasing drought intensity and woody encroachment, a process that results in increased woody plant abundance and decreased herbaceous plant abundance. Reduced soil moisture and shifts from herbaceous to woody plant dominance are likely to alter C pools in the soil. Our project combines observational, experimental, and modeling approaches to project ecosystem consequences of woody encroachment in the central Great Plains region.

Complex interactions between root inputs, water loss, and C pools were evident when comparing belowground C pools among plant cover types. A shift from grassy to woody cover resulted in an increased soil C pool, mostly notably at 50-100 cm deep. Priming occurred in grassy, but not woody soils, and grass-derived SOM was more available than woody-derived SOM. We used large rain-out shelters to reduce water availability for shrubs and grasses growing in annually and infrequently burned (every 4-yr) locations. In general, physiological and morphological responses to reduced rainfall were less pronounced than responses to fire frequency. For the first two years of this project, leaf gas exchange rates, water potential, and turgor loss point were lower in the woody encroached 4-yr burn treatments. Stable isotopic analyses of xylem water in shrubs in 4-yr burn treatments had lower values; indicative of water use from deeper soils depths. Deeper-water reliance by the shrubs buffered seasonal photosynthetic variability and mitigated water stress compared to grasses that showed greater reliance on surface soil moisture.

Fine root length and biomass in surface soils (0-25 cm) was highest under grassy cover compared to woody, and generally declined with increasing fire frequency. At greater depths (25-100 cm), fine root biomass was relatively low (< 1 g/cm^3) under all cover types and burn treatments. Drought reduced the ability of grass roots to move water but had no impact on shrub

roots. Shrub roots were less vulnerable to water stress when grown under drought compared to control conditions.

Finally, these data have been used to parameterize a numerical terrestrial ecosystem model (the Functionally Assembled Terrestrial Ecosystem Simulator, FATES) for the Konza Prairie. Preliminary results indicate that our calibration of the model can accurately represent vegetation responses to frequent fire for both shrub and grass functional types.

Automated Chambers in a Tidal Wetland Collect High-Frequency Methane Measurements

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Project Lead Principal Investigator (PI): Genevieve Noyce

BER Program: ESS

Project: University Project

Due to the dynamic nature of the coastal Terrestrial-Aquatic Interface (TAI), the processes that regulate decomposition are of greater significance at the TAI than in upland systems, especially because decomposition in anaerobic environments is accomplished through multiple interacting microbial processes that influence carbon storage and emissions of greenhouse gases, including methane (CH_4). However, we have little knowledge of how climate stressors such as salinity, inundation, and warming interact to drive CH_4 cycling and other decomposition processes, even though accurately modeling these processes is critical for incorporating the coastal TAI into Earth systems models. Our past modeling and experimental work has highlighted that we need more information on the processes that couple climate stresses, decomposition pathways, and net primary productivity in order to characterize feedbacks between biological, physical, and biogeochemical processes, and also to identify, and thus model, heterogenous soil conditions that lead to "hot spots" or "hot moments".

In coastal wetlands, tidal and precipitation events can contribute to "hot moments" of CH_4 emissions, but these events are easily missed with typical chamber sampling frequency. To address this problem, we installed a network of 12 automated chambers in the Smithsonian's Global Change Research Wetland in spring 2021. The sampling system is controlled by an LGR Ultraportable Greenhouse Gas Analyzer and two multiplexers. Every 6 minutes, one chamber automatically closes and collects a 5-minute measurement of CH_4 and CO_2 emissions or uptake, leading to 240 flux measurements per day. An AquaTROLL 200 continuously measures water level and salinity for the entire site. Inside the chambers, a network of low-cost DIY I^2C sensors measure CO_2 (K30 from Sensaire), air temperature, humidity, and pressure (BME680 chip), and soil temperature at 10 and 25 cm (thermistors) at 10 second intervals. All data streams are sent to CR1000 loggers and synchronized for downstream analysis. Using this system, we can identify high flux events and start to pinpoint the environmental conditions that lead to their occurrence.

Title: **Loading of Dissolved Organic Carbon to Western Arctic Rivers from Process-Based Modeling**

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Project Lead Principal Investigator (PI): Michael Rawlins

BER Program: TES

Project: University Project

Project Abstract:

The mobilization and land-to-ocean transfer of dissolved organic carbon (DOC) in Arctic watersheds is intricately linked with the region's climate and water cycle, and furthermore at risk of changes from climate warming and associated impacts. This study quantifies model-simulated estimates of runoff, surface and active layer leachate DOC concentrations and loadings to western Arctic rivers, specifically for basins that drain into coastal waters between and including the Yukon and Mackenzie rivers. Model validation leverages data from other field measurements, synthesis studies, and modeling efforts. The simulations effectively quantify DOC leaching in surface and subsurface runoff and broadly capture the seasonal cycle in DOC concentration and mass loadings reported from other studies that use river-based measurements. A marked east-west gradient in simulated spring and summer DOC concentrations of 24 drainage basins on the North Slope of Alaska is captured by the modeling, consistent with independent data derived from river sampling. Simulated loadings for the Mackenzie and Yukon show reasonable agreement with estimates of DOC export for annual totals and four of the six seasonal comparisons. Nearly equivalent loading occurs to rivers which drain north to the Beaufort Sea and west to the Bering and Chukchi Seas. The modeling framework provides a basis for understanding carbon export to coastal waters and for assessing impacts of hydrological cycle intensification and permafrost thaw with ongoing warming in the Arctic.

Title: **Influence of hyporheic exchange on coupled S-Fe-C biogeochemical cycling and microbial community function in riparian wetlands at the Savannah River Site**

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BER Program: ESS

Project: University Project

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

In the uncontaminated area of Tims Branch at the Savannah River Site, we have set up a number of subsites with continuous surface- and ground-water level and flux measurements. These sites vary in terms of flux direction and magnitude throughout the year, with visible cues of flux direction from the presence or absence of Fe-oxidize encrusted microbial mats in gaining or losing stream conditions, respectively. There is a high concentration of Fe in the sediment porewaters and sediments that varies seasonally and sulfide measurements were very low at all times of the year sampled. 16S rRNA gene sequencing was performed on sediment cores collected in January and August 2019 to characterize the spatial and temporal microbial community distribution. The overall microbial community was similar between the two seasons except for changes in the relative abundance of phyla with depth. Preliminary functional group analysis suggests a greater relative abundance of S cycling orders at gaining stream subsites relative to losing stream locations. Although it is unclear why, some subsites further downstream

that experience occasional flooding due to beaver damming had a much higher relative abundance of methanogenic orders than other sites. Correlations between geochemical parameters and microbial community, visualized through non-metric multidimensional scaling (NMDS) ordinations, revealed that the microbial community in losing stream sediments were most dissimilar to gaining stream sites, indicated that hyporheic fluxes impact microbial community structure. Metagenome analysis underway will help us further understand the spatial and temporal taxonomic and functional affiliations at these sites.

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

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BER Program: EES

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

Project Abstract: Wetlands and hyporheic zones are critical interfacial regions with complex and seasonally-varied dynamics in hydraulic, chemical, physical and microbial properties, which result in their functioning as a sink or source of organic matter (OM) and associated contaminants, such as uranium (U). Molecular-scale understanding of the interactions between OM and U under seasonally-varied hydrological conditions (water table height, nutrients, surface water recharge and discharge inferred by ^{2}H and ^{18}O) in these critical zones is needed to fully resolve the regulating processes which are crucial for incorporation into watershed reactive transport models. Our **central hypothesis** is that ***watershed interfacial zones, including wetlands and hyporheic zones, produce unique yet characterizable OM, with seasonal variabilities in both quantities and qualities, which are controlled by watershed hydrology/events. This seasonal, hydrological processes-driven OM dictates uranium binding and transport patterns in the long-term stewardship sites of the DOE complex***. To address this hypothesis, we are first addressing the following set of questions through field-oriented studies at the Argonne Wetland Hydrobiogeochemistry SFA field site (a U-contaminated wetland of the Savannah River Site) and accompanying laboratory experiments: 1) What is the optimal method(s) to differentially extract stable (immobile) versus mobile natural organic matter (NOM) from the same sedimentary or aquatic sample? We developed a method capable of differentially extracting immobile and mobile NOM fractions (high-molecular-weight and low-molecular-weight components for each) that are suitable for molecular-level chemical characterization via Fourier-transform ion cyclotron resonance mass spectrometry (FTICR-MS). 2) How does NOM composition impact the physical properties (e.g., hydrophobicity) underlying their aggregation/disaggregation behavior? How do diagenetic processes affect the massive occurrence of flocs in the gaining stream and the scavenging of U? We observed NOM concentrations (as calculated as the sum of carbohydrates and proteins in mg-NOM/g-particles) increasing

in the order of floc > suspended particulate matter (SPM) > bottom sediment; whereas, the protein-to-carbohydrate ratio (an index for stickiness for aggregation) was in the order of SPM > flocs > bottom sediment. Flocs contained 4 to 5-fold higher U than the stream bottom sediment. 3) What is U distribution in a dynamic watershed with relevance to groundwater-surface exchange? 4) What role does sedimentary phosphorus speciation play in U distribution in this watershed? Information from this project will identify and quantify important hydrologically driven biogeochemical processes impacting uranium at this SFA.

Coupled Long-Term Experiment and Model Investigation of The Differential Response of Plants and Soil Microbes in a Changing Permafrost Tundra Ecosystem

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Project: University
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Project Abstract:
There are 1460-1600 billion tons of soil carbon in the northern circumpolar permafrost region, more than twice as much carbon than in the atmosphere. Understanding the magnitude, rate, and form of greenhouse gas release to the atmosphere is crucial for predicting the strength and timing of this carbon cycle feedback to a warming climate. Here we report results from an ecosystem warming manipulation where we increased air and soil temperature, and degraded the surface permafrost. We used snow fences coupled with spring snow removal to increase deep soil temperatures and thaw depth (soil warming) and open top chambers to increase growing season air temperatures (air warming). The soil warming treatment has successfully warmed soils by 2-3ºC in winter, has increased growing-season depth of ground thaw by up to 50%, and has degraded an increasing amount of surface permafrost each year of the project. To determine the impact of subsidence on permafrost thaw and soil carbon, we quantified subsidence using high-accuracy differential GPS over the course of the experiment. With permafrost temperatures already near 0°C, almost 11 cm of subsidence was observed in control plots over 9 years. Experimental air and soil warming increased the amount of subsidence five-fold and also created inundated microsites as the subsided soil surface was closer to the water table. Across treatments, the loss of ground ice was responsible for 85-91% of the subsidence, while 9-15% of the subsidence was linked to the loss of organic matter. Accounting for subsidence, permafrost thaw was 19% (control) and 49% (warming) deeper than active layer thickness measurements alone would have indicated. This corresponds to 37% (control) and 113% (warming) more carbon in the newly thawed active layer as compared to the beginning of the experiment. Radiocarbon measurements of ecosystem respiration indicated that wetter soils may limit the decomposition of old organic matter emerging from permafrost. In 2018, soil drying resulted in a 30-fold increase in old soil contribution to ecosystem respiration as compared to the wet years 2016 and 2017. In the dry year, old soil contributed up to 39% of total ecosystem respiration. Improved model structure that includes the physical subsidence of ground, or parameterizations that capture such effects, may be needed in order to capture the non-linear dynamics revealed by this unique long-term experiment.

Integration of Omics into a New Comprehensive Rate Law for Competitive Terminal Electron-Accepting Processes in Reactive Transport Models: Application to N, Fe, and S in Stream and Wetland Sediments

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Project: University Project

Project Abstract: The dynamic of biogeochemical processes in sediments and their role in carbon transformation cannot be predicted accurately by current reactive transport models (RTMs). These models largely rely on detectable changes in geochemical conditions to activate metabolic processes, do not accurately describe microbial competition, and poorly constrain the effect of hydrological perturbations on biogeochemical processes. The objectives of this project are to: (i) develop new rate laws for RTMs that rely on a combination of high throughput omics (meta-genomic, -transcriptomic, -proteomic, -bolomic) and geochemical signatures to identify the underlying anaerobic microbial processes in stream and wetland sediments; (ii) describe the competition between the dominant metabolic processes; and (iii) quantify carbon transformation under varying hydrological conditions. A combination of meta-omic and geochemical signatures identified the main anaerobic microbial processes in a Savannah River Site (SRS) wetland and Oak Ridge East Fork Poplar Creek (EFPC) sediment. Geochemical depth profiles suggested that Fe(III) reduction dominates biogeochemical processes in SRS wetland sediments, whereas a combination of NO_3^- and Fe(III) reduction dominates EFPC sediments. Sediment slurry incubations designed to investigate the competition between anaerobic microbial processes demonstrated that NO_3^- reduction was the fastest respiratory process and that Fe(III) reduction became dominant once NO_3^- was depleted. Incubations also revealed that SO_4^{2-} reduction was inhibited by Fe(III) reduction and that this inhibition was enhanced by ferrihydrite addition. Metagenomic signals were enriched in gene variants indicating that bacteria couple anaerobic $\sum H_2S$ oxidation to NO_3^- reduction in EFPC but not SRS sediments. Metagenomic data thus indicate that a cryptic sulfur cycle may be more significant than apparent by geochemical signals in EFPC sediments. Geochemical and genomic data of SRS incubations instead point towards

outcompetition of sulfate-reducing bacteria for carbon substrate by iron-reducing bacteria. The metagenomic data is currently being confirmed via complementary meta-transcriptomic and -proteomic analyses. A gene-centric kinetic model was developed with new rate laws to account for competition between microbial communities. The model calibrated with one set of incubations was able to reproduce all SRS incubation treatments and indicated carbon substrate competition as the main control of anaerobic metabolic processes. Overall, this project demonstrates that: (i) a combination of high throughput omic and geochemical data is needed; and (ii) simple gene-centric models can be readily included in RTMs to accurately identify biogeochemical processes and microbial community competition in sediments. The role of hydrological processes on sediment biogeochemistry in gaining and losing stream SRS sediments is currently being characterized.

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

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Project: University led project
Project Abstract:
The existing paradigm describes oxidation of reduced chemical species, such as Fe(II) and U(IV), following an influx of oxidants such as dissolved oxygen (DO) or nitrate. However, prior field results challenged current understanding of the oxidant's role controlling redox behavior of metals/radionuclides; low concentrations of an oxidant (DO) injected into a biostimulated reduced region of an alluvial aquifer stimulated a decrease in aqueous U concentrations *in situ*. Here we experimentally test the impact of a highly soluble oxidant, nitrate, on U redox state using organic-rich, naturally reduced-U bearing oxbow lake sediments (collected from Riverton, WY; SLAC SFA). Triplicate batch reactors of reduced sediments were amended with anoxic bicarbonate buffered medium with and without the addition of nitrate at varying concentrations (low nitrate <14 mg/L-N> high nitrate) following preincubation with added uranyl chloride (final concentration 5 mg/L). High nitrate amended batch reactors increased dissolved U(VI) consistent with oxidation of reduced species. However, low nitrate amendments resulted in a decrease of dissolved U(VI), consistent with reduction. No significant change in dissolved U(VI) was observed in controls amended with anoxic DI water. XANES analysis of collected sediments revealed an increase in sedimentary U(IV) (85% of U) in reactors amended with low nitrate relative to the control (40% U(IV) of sedimentary U). Thus indicating U(VI) reduction in response to low nitrate amendment. An increase in aqueous Fe(II) further supported the onset of reducing conditions. A decrease in sulfide was observed. PHREEQC modeling of geochemical data indicated Fe-sulfide precipitation, which would account for the observed decrease in aqueous sulfide. Reduction activity in low nitrate amended treatments occurred concurrent with an increase in dissolved organic carbon (DOC) and cell and virus abundance. Metagenome assembled genomes revealed the metabolic potential for both lithotrophic and organotrophic nitrate reduction as well as metal/radionuclide and sulfur cycling. Recovery of metagenome assembled virus genomes from microbial (>0.2μm) and virome (<0.2 μm and >0.05 μm) samples indicated a change in viral community in response to nitrate amendments. These results indicate the potential of microbially-mediated cell lysis and recycling of organic carbon. To verify that the observed geochemical processes were stimulated by microbial activity, batch reactors were amended with the antibiotic chloramphenicol and demonstrated suppression of both nitrate reduction and removal of aqueous U. Together these results demonstrate that in organic rich sediments a "tipping point" exists where an influx of an oxidant can lead to the increase in DOC supporting microbial activity and reducing conditions.

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

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Project: University Project (Whitman Lab)

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Project Abstract: Boreal forests hold between 370-1720 Pg carbon (C) above- and belowground, making them a major stock of C globally. In North American boreal ecosystems, wildfire is the primary stand-replacing disturbance, and fires are projected to increase in frequency and severity in the future, which could affect soil C cycling and microbial community composition. However, data quantifying these effects are sparse, and our understanding of the mechanisms driving them remains limited. Recent advances in biogeochemical model representations of soil C cycling, such as the Carbon, Organisms, Rhizosphere and Protection in the Soil Environment (CORPSE) model, have included an emphasis on explicitly representing the system in an increasingly mechanistically accurate way. In our project, we aim to determine whether linking belowground microbial community composition, size, and activity to aboveground properties of burn severity and plant community composition (upland jack pine and upland spruce) allows us to better model post-fire soil CO_2 fluxes using the CORPSE model.

Our first project objective is to quantify changes in C fluxes, microbial biomass, and microbial community composition, after simulated fires in intact soil cores across a burn severity gradient. Here, we present our initial findings related to this objective. Using a cone calorimeter, we simulated wildfires in intact soil cores, manipulating soil moisture to achieve lower and higher burn severities. We incubated burned and unburned control soils for up to six months, tracing CO_2 emissions using KOH traps and characterizing soil microbial community composition using high-throughput sequencing. Higher severity burns generally resulted in greater C losses but lower C:N ratios, greater increases in soil pH, and smaller fast-cycling C pools in a simple two-pool exponential decay model than lower severity burns. Higher severity burns were also accompanied by greater shifts in bacterial community composition, including a shift toward taxa with higher predicted weighted mean 16S rRNA gene copy numbers – a parameter associated with the potential for fast growth.

Future objectives will include developing and evaluating adaptations to the CORPSE model to better represent post-fire SOC dynamics along a burn severity gradient across a hierarchy of model complexity and testing the capacity of the adapted CORPSE model to predict CO_2 flux rates in burned cores from new sites.

Title: **Coupling streambed dynamics with nutrient and fine sediment transport in mountainous watersheds**

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BER Program: ESS

Project: University Project

Project Abstract: In mountainous watersheds, rivers typically have an armor layer of coarse sediment that protects the finer subsurface from erosion. Armor layer motion during high magnitude flows releases the fine sediment present in the subsurface layer, which may be enriched in Phosphorus (P) and Particulate Organic Carbon (POC). Therefore, armor layer transport could explain temporal variations in POC, suspended sediment (SS), and various forms of P exported from many watersheds. In addition, streambed concentrations of these constituents may depend on whether a reach is losing or gaining. We are currently measuring armor layer motion, as well as streambed and river concentrations of POC, P, and fine sediment using detailed field measurements in two reaches (one gaining, one losing) in La Jara Creek in Valles Caldera National Preserve, NM. Our measurements will occur over two summer monsoon and two snowmelt seasons to document temporal changes in armor layer motion, streambed nutrient and sediment release, and surface and groundwater exchange. We have completed field instrument installation and have started our first monsoon season of monitoring. Our study addresses 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.

Linkages Between Hydrologic Processes and Biogeochemical Cycling in Salt Marshes

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Salt marshes exist at the terrestrial-aquatic interface between watersheds and the ocean. These tidal systems are hot spots of biogeochemical activity within coastal watersheds. Yet, we have limited understanding regarding how short-term (e.g. daily tidal cycles) and long-term (e.g. seasonal precipitation and climate patterns) hydrologic forcings may interact within these systems. These interactions will affect the temporal dynamics, or hot moments, of nutrient processing as well as the physical zonation of biogeochemical processing in the subsurface, or hot spots. To address this knowledge gap, we instrumented a ~25 m transect along a representative salt marsh platform at the Elkhorn Slough National Estuarine Research Reserve in California, USA. We installed variable-depth redox probes, nested piezometers, and a field-deployable spectrophotometer with a multi-source pump at lower, mid, and upper marsh positions to allow for characterization of subsurface hydrologic cycling and dissolved inorganic nitrogen (DIN) species concentrations at a high frequency (~15 min). We also conducted seasonal sediment incubation experiments to quantify nitrogen processing rates. We found that DIN concentrations fluctuated hourly due to frequent tidal flushing that introduced oxygen and ammonium-rich surface water into sediments under reduced conditions, with the largest change in concentrations observed in lower marsh positions. Sediment core incubations showed a dominance of net N_2 flux out of the marsh, indicating removal by denitrification, but the impacts of seasonal and event-driven freshwater contributions affected elevations differently, with the largest changes seen in upper marsh positions. Together, our findings suggest that intra-annual changes in source water contributions across the marsh result in functional zonation, where lower marsh position functions may be regulated by tidal flushing and upper marsh position functions may be regulated by freshwater contributions.