

**2019 ENVIRONMENTAL SYSTEM
SCIENCE PRINCIPAL INVESTIGATORS
MEETING
ABSTRACT BOOK**

April 30 - May 1, 2019
Bolger Center, Potomac, MD

2019 Environmental System Science Principal Investigators Meeting

April 30 – May 1, 2019

Organized by the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research

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Table of Contents

(Click on any line to advance to the abstract)

Environmental System Science

[Student Abstracts](#)

[Early Career Research Program Awards](#)

Terrestrial Ecosystem Science

[University Awards](#)

[Next Generation Ecosystem Experiments \(NGEE\): Arctic](#)

[Next Generation Ecosystem Experiments \(NGEE\): Tropics](#)

[AmeriFlux Management Project](#)

[Argonne National Laboratory Science Focus Area](#)

[Lawrence Berkeley National Laboratory Science Focus Area](#)

[Oak Ridge National Laboratory Science Focus Area](#)

[Pacific Northwest National Laboratory Project](#)

Subsurface Biogeochemical Research

[Argonne National Laboratory Science Focus Area](#)

[Lawrence Berkeley National Laboratory Science Focus Area](#)

[Lawrence Livermore National Laboratory Science Focus Area](#)

[Oak Ridge National Laboratory Science Focus Area](#)

[Pacific Northwest National Laboratory Science Focus Area](#)

[SLAC Science Focus Area](#)

[IDEAS-Watersheds Project](#)

[University Awards](#)

[Scientific User Facilities and Community Resources](#)

[Small Business Innovative Research Awards](#)

Environmental System Science

Student Abstracts

Poster #1-1**Nitrogen Fertilization Increases Carbon Use Efficiency of Soil Microbial Communities Across 10 Long-term N Fertilization Studies**

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BER Program: TES

Project: Student Travel Award

Soils store more carbon (C) than both the atmosphere and vegetation combined. Thus, any changes in the rate at which soil microbes release CO₂ into the atmosphere through respiration has critical implications for atmospheric CO₂ concentrations and ultimately Earth's climate. Historically, N deposition has altered the decomposition of soil C in temperate forests. While most studies show reduced decomposition of soil C under long-term N fertilization, the underlying mechanisms that drives this reduction remain unclear. We hypothesized that elevated soil N as the result of N fertilization may reduce the need for microbes to mine N from soil organic matter (SOM) resulting in a community shift that favors microbial scavengers over miners. As such, there is a greater return on extracellular enzyme investment, higher microbial carbon use efficiency (CUE) and enhanced production of microbial necromass. Given that microbial necromass is the precursor of stable SOM, these shifts in CUE and turnover may also contribute to greater soil C protection. To test this hypothesis, we measured microbial community CUE in fertilized and control plots across ten long-term N fertilization experiments spanning Eastern temperate forests. We incubated soils in the lab with ¹³C labelled glucose and measured the fraction of this substrate released during respiration vs. what was incorporated into microbial DNA. We found that long term N fertilization increased microbial CUE as respiration of ¹³C glucose was lower in N fertilized soils along with greater incorporation of ¹³C into DNA. Moreover, we found that N deposition enhanced microbial turnover. Collectively, our results suggest that shifts in CUE and turnover may be an important mechanism that explains reduced soil respiration across N fertilization studies as well as enhanced soil C stocks, owing to microbial necromass being the primary precursor of stable SOM.

Poster #21-14**Impacts of Transient Hydrologic Conditions on Metal and Carbon Cycling in the East River Floodplain**

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Project: Student Travel Award

My research contributes to two DOE-funded projects: a university project (Stanford University) and a subproject of the LBNL Watershed Function SFA. The goal of the university project is to understand principal controls on carbon cycling in floodplains, while the goal of the SFA subproject is to understand the impact of floodplain sediments on river chemistry. My specific objective is to determine the impacts of transient hydrologic conditions (seasonal snowmelt, beaver dam construction) on exports of carbon and metals from meander sediments to the East River. My work toward this goal consists of: (1) instrumenting three-dimensional well-fields for hydrologic and biogeochemical characterization of meanders, and conducting high-frequency sampling of river, groundwater, and sediments at these sites; and (2) developing reactive transport models of meanders - including calibration and validation. Not only has this work led to an understanding of the processes controlling carbon and metal exports from floodplain sediments and their sensitivity to hydrologic transients, it also facilitates quantification of the effluxes of carbon and metals from the sediments to the river. Furthermore, the combination of fieldwork and modeling has revealed that oxidizing and reducing zones are spatially and temporally distributed in floodplain, and that these distributions act as a central control on fluxes of dissolved metals and carbon into river waters.

My research over the last two years centered on two summers (2017, 2018) of fieldwork at East River. This work is essential for both the university project and the SFA subproject, and includes installation of piezometers for groundwater sampling, rhizons for sampling pore-water from the unsaturated zone, and pressure transducers for recording groundwater levels. Surface and groundwater samples were collected for measurement of pH, electronic conductivity, redox potential, and temperature. Further, sediment cores were collected and examined for organic matter and metal chemistry. This summer (2019) will be my third field season in the East River area, continuing my examination of floodplain processes driving biogeochemical cycling of carbon and metals and their export into river waters.

Alongside fieldwork, I developed 2D and 3D reactive transport models (PFLOTRAN) of meanders posited to be hotspots of reactivity. With the models (validated with the high-resolution temporal and spatial data collected over multiple field seasons) I quantitatively integrated the hydrologic and biogeochemical processes in the meanders. The models facilitate quantification of carbon and metal fluxes from meander sediments to the river, and they reveal the sensitivity of the processes controlling fluxes to hydrologic changes.

Poster #21-68**Effect of Hydropeaking Operations on Hyporheic Zone Thermal Regime**

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Project: Student Travel Award

Hydropeaking, the alternating storage and release of water from reservoirs for the purpose of hydropower generation, perturbs the thermal regime of many large rivers. While the effects of hydropeaking, and more broadly all types of hydropower operations, on stream thermal regimes have been long studied, there is a paucity of work on how dam operations impact the thermal regime of the streambed hyporheic zone. Streambed temperature is an important control on both biotic (N, C) and abiotic (metals) constituents as well as habitat suitability for benthic organisms (invertebrates, fish eggs, and microbial populations). Thus, developing a more complete understanding of how frequent river fluctuations from dam operations affect the streambed thermal regime will enable more comprehensive characterization and prediction of the effects of dam operations on river ecosystems.

This study uses a novel field dataset combined with numerical modeling to investigate hydropeaking's impact streambed thermal regime in a large regulated river. The field data was collected from the 4th order Lower Colorado River at a site 12 km downstream from a dam that induces large daily flow variations. We used 24 vertical thermistor arrays to obtain time series data of streambed temperatures in the shallow 50 cm of streambed across the entire ~70 m channel. The data was collected over 7 days of continuous daily flow oscillations. Our field data revealed two distinct regions in the streambed. The near-bank areas of the streambed were highly dynamic thermally, transitioning between river and groundwater temperatures on a daily basis. This was in contrast with the rest of the streambed located away from the bank where the thermal regime was more similar to that of the river.

To aid in the interpretation of the field observations and to provide a more general explanation of the observed phenomenon, we ran 2-D fluid flow and heat transport models for a river channel subjected to the same forcings as our study site and with similar hydraulic properties. We additionally explored the effect that hydraulic conductivity and groundwater conditions have on the formation of the two distinct regions observed in the field data. Our modeling results demonstrate that strongly gaining groundwater conditions and high hydraulic conductivity favor the development of thermally dynamic zones near river banks, while low hydraulic conductivity and/or gaining groundwater conditions result in more muted temperature fluctuations. These patterns could help predict thermally sensitive processes in the streambeds of hydropeaked or flooding rivers.

Poster #1-2**Comparison of Microbial Parameters Parameterized based on Short-term and Long-term Incubation**

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Project: Student Travel Award

In the Microbial-Enzyme Decomposition (MEND) model, five microbial parameters relevant to microbial uptake, growth, maintenance and dormancy are critical to model performance but are usually parameterized based on short-term measurements. These parameters include the initial active fraction of microbes (r_0), maximum specific growth rate (V_g), a ratio (α) between maximum specific maintenance rate (V_{mt}) to the sum of V_{mt} and V_g , half saturation constant of dissolved organic carbon uptake (K_D) and true growth yield (Y_g). To assess how model projection of soil C stock vary with parameterizations based on measurements over different time scales, this study compared modelled soil responses to 5°C warming by implementing best-fit parameters calibrated based on soil incubation datasets over 144 hours and 729 days (referred to as short-term or ST parameters, and long-term or LT parameters). Results showed that all five best-fit ST parameters were higher by 7.7~420% than LT parameters. Under 5°C warming, model projected significant steady-state SOC loss ($-15.4 \pm 0.1\%$) and minor SOC gain ($2.1 \pm 0.2\%$) using ST and LT parameters, respectively. Compared to meta-analysis synthesis, LT parameters projected more realistic SOC response to long-term warming. MEND analytic steady state solution demonstrated that the relative change of SOC under warming depended upon Y_g only, so the overestimate of SOC losses to warming using ST parameters were attributed to higher best-fit Y_g . This study suggests that to improve the accuracy of long-term SOC projections, parametrization of microbial relevant processes particularly true growth yield, should be achieved relying upon measurements over long time scale.

Poster #1-3**Inter-annual Variation in Radiocarbon Age of Ecosystem Respiration over Ten Years of Permafrost Warming**

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Project: Student Travel Award

Permafrost carbon (C) has accumulated in northern latitudes throughout the Holocene because of frozen and waterlogged conditions. As air temperatures increase with climate warming, we expect to see an increase in permafrost thaw and a decrease in environmental constraints on microbial decomposition. Over decadal timescales, highly thawed permafrost areas can release more old C than minimally thawed areas. Since the bulk of permafrost C is old, we anticipate that long-term C losses will largely originate from both old and slowly decomposing C pools. Our study was conducted in a moist acidic tundra site near Eight Mile Lake, Alaska where we have experimentally warmed permafrost for a decade, and tripled the rate of thaw relative to control. We utilized natural abundance $\Delta^{14}\text{C}$ as a tool to estimate the age of ecosystem respiration (Reco) during the peak of the growing season, from 2009 to 2018. My contributions to this long-term dataset included the collection of CO_2 samples in 2011, 2013, 2014, 2017 and 2018, and data analyses. We found that Reco $\Delta^{14}\text{C}$ decreased at a rate of 12‰ per year (CI: -23 to -0.4‰ year⁻¹) in both control and soil warmed plots. However, soil temperatures at 40 cm induced a slower rate of decrease in Reco $\Delta^{14}\text{C}$ in soil warmed plots relative to control by 3‰ over time (CI: 0.3 to 6‰). This phenomenon may be attributed to warmer temperatures increasing plant activity and C input to soil with contemporary (more enriched) $\Delta^{14}\text{C}$ values, which can dilute the isotopic signal of old C, even when its contribution to Reco increases. In some years, we observed substantially more negative Reco $\Delta^{14}\text{C}$ values across all treatments, indicating high rates of old soil C loss to the atmosphere. Since permafrost regions have historically been C sinks, an increase in soil C flux to the atmosphere has large implications for the net ecosystem C balance in the Arctic. If permafrost regions become a C source to the atmosphere, the effects of climate warming could be exacerbated.

Poster #21-53**NpO₂(s) Dissolution Under Vadose Zone Conditions**

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Project: Student Travel Award

A novel field experiment at Savannah River Site (SRS), the Radionuclide Field Lysimeter Experiment (RadFLE_x), is the basis of investigation of neptunium migration and geochemical behavior in the vadose zone. These studies probe the effect of oxidation state on neptunium transport, the effect of source characteristics on release mechanisms, and the effect of colloids on transport. With a long half-life and potentially high environmental mobility, neptunium geochemistry is of paramount importance for risk assessment and environmental health and safety, but field-scale evidence of neptunium transport from sources of varying oxidation state has yet to be reported. The specific release from NpO₂(s) is of interest because typical conceptual models based on uranium oxidation would predict surface oxidation of neptunium oxide as a rate-limiting step in transport of neptunium away from the source region.

Field data indicated that downward migration of Np from a NpO₂(s) source was due to transport of 1) soluble neptunyl, NpO₂⁺ ions and 2) eigen colloids of NpO₂(s). Both mobile species were proposed to be formed during oxidative dissolution of NpO₂(s). Based on these observations, a hypothesis for new experiments was developed wherein dissolution of polycrystalline phases occurs via alteration of phases along grain boundaries and formation of mobile colloids or polynuclear aqueous species. New NpO₂(s) sources were placed in lysimeters and three depths and exposed for one year. Electron microscopy verified alteration of NpO₂(s) through formation of granules along grain boundaries (Figure 1). Complimentary laboratory-based dissolution studies were initiated under vadose zone conditions (~pH 5, oxic conditions), used to mimic environmental conditions the source was exposed to in field lysimeters. Both aqueous and solid phases are monitored to identify the rate and mechanisms involved in NpO₂(s) dissolution.

This work is motivated by a lack of dissolution studies of NpO₂(s), particularly non-hydrated or amorphous phases, at environmentally relevant conditions. Specifically, there is a need for greater understanding of the mechanisms of NpO₂(s) dissolution, including grain boundary formation, relative importance of presence of oxygen and water on grain boundary formation and dissolution, rates of dissolution in presence and absence of oxygen, and potential impact of colloidal species. Overall, these efforts seek to validate observed field data and bridge understanding of NpO₂(s) dissolution from field to nano scale.

Poster #1-4**Effects of Phenotypic Diversity on Litter Decomposition are Contingent on Linked Traits**

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BER Program: TES and Genomic Sciences

Project: Student Travel Award

Soil microbial communities show considerable differences in how their metabolisms respond to elevated temperatures, with some communities becoming more conducive to carbon storage, while others become less-so. Carbon use efficiency (CUE) - or the fraction of carbon taken up by a cell and incorporated into biomass and biomass products rather than being respired – is often cited as a key determinant of the intermediate longevity of soil carbon stocks. However, soil carbon cycling models fail to include the diversity of carbon use efficiency responses to temperature, so their effects are unknown. Therefore, we evaluated how incorporating taxon- level variability of CUE temperature responses into DEMENT affected on the local carbon cycle. The trait-based DEMENT model was chosen because it enables explicit organism-level tradeoffs and is therefore conducive to the introduction of diverse physiology.

Each taxon in the model was assigned a temperature sensitivity of CUE between -0.022 and $+0.022^{\circ}\text{C}^{-1}$, and the outputs of this “variable CUE” scenario were compared for simulations run at 15 and 20 °C. An additional run where all taxa were assigned the cross-taxon mean of the first (ie 0°C^{-1}) was generated as a comparison. We found that warming led to rapid litter loss (37%) when CUE temperature response was allowed to vary among taxa, and that this was associated with a 47% larger microbial biomass pool over the first 5000 days. By contrast, warming led to just a 14% greater litter loss when temperature response was fixed. However, this conclusion was contingent on the relationship between the resources taxa allocate to extracellular enzyme production. Forcing taxa with greater decomposition potential to have a more positive growth efficiency response to warming selected for a smaller community enriched in extracellular enzymes and even greater litter loss (67%). However, forcing the carbon use efficiency of taxa with more enzymes to respond less favorably to temperature did not cause warming-induced losses of litter carbon.

As such, considering intertaxon variability in CUE temperature response led to changes in litter decomposition with warming which differed from that expected with a homogenous response under this model. This builds on the growing cognizance of the importance of explicitly considering the physiological ecology of soil microbes with respect to the carbon cycle, rather than some average.

Poster #21-69**More than Meets the Eye: Microbial Communities and their Viral Predators Govern Carbon and Nitrogen Transformations in the Hyporheic Zone**

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BER Program: SBR

Project: University award

Microorganisms are catalysts for carbon and nitrogen geochemical cycles in hyporheic regions of river sediments, yet the microbial metabolisms underlying these processes are largely unknown. Moreover, the viral ecology impacting these microbial nutrient cycles in river sediments is to a great extent unexplored. Here, we performed metagenomic and metaproteomic analyses on 6 sediment cores, with samples collected at 10 cm intervals from the surface down to 60 cm below the surface. We reconstructed 67 near-complete genomes from the 5 most abundant and active microbial lineages including members of Nitrospirae, Thaumarchaeota, Firmicutes, Proteobacteria, as well as members from 6 other phyla. Genome metabolic inferences indicated that ammonium is a central metabolite connecting all organisms in this system. Expression data confirmed that organic nitrogen degradation (e.g. peptides and amino acids) by Proteobacterial and Firmicutes members provides a source of ammonium to the system. One of the most dominant and active community members, the Thaumarchaeota (renamed to Crenarchaeota), oxidize ammonium into nitrite. Subsequent nitrite oxidation by members of the Nitrospiraceae could fuel denitrification by members of the Proteobacteria, ultimately yielding nitrogen gas production, including nitrous oxide. Evidence for heterotrophic carbon oxidation (e.g. phenolics) results in the generation of simple sugars and carbon dioxide, the latter of which can be consumed by autotrophic nitrifiers. Consistent with our proteomic data, chamber and porewater measurements demonstrated that nitrous oxide and carbon dioxide fluxes respond to river stage and the greatest nitrous oxide concentrations were near the sediment surface. Our viromic analyses recovered 412 unique viral populations, several of which may contribute to carbon and nitrogen cycling in this system. *In silico* predictions linked a 19 kb viral genome to 3 Thaumarchaeota genomes, suggesting viral predation of active nitrogen cycling microorganisms. Viruses also encoded carbohydrate and amino acid degradation auxiliary metabolic genes, indicating viral influence of carbon degradation and ammonium formation, respectively. Together these genome enabled predictions uncover microbial and viral roles contributing to interdependent carbon and nitrogen fluxes from river systems.

Poster #1-5**Warming Effects on Litter Decomposition and Soil Respiration in a Tropical Forest**

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BER Program: TES

Project: Student Travel Award

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

Litter decomposition and soil respiration are important ecosystem processes in tropical forests, and their responses to ongoing changes in climate will have important consequences for the global carbon cycle. The Tropical Responses to Altered Climate Experiment (TRACE) in Puerto Rico investigates how tropical forest ecosystems will respond to increased temperatures. The TRACE field site has six plots, three controls at ambient temperature and three warmed at 4°C above ambient temperatures. Working with TRACE, we evaluated the effects of sustained warming on 1) in-situ litter decomposition and 2) *ex-situ* soil respiration. For the in-situ litter decomposition, we measured rates of decomposition across four substrates (native litter, green tea, black tea and wood) over a three-month period. Contrary to our hypothesis that increased temperatures would increase litter decomposition rates, we found that warming reduced mass loss by an average of ~10% across the four substrates. Warming decreased soil and litter moisture by an average of ~35%, which limited microbial activity and decomposition. However, the effect of warming on reduced mass loss varied among the different substrates (green tea: not significant, native litter: 3% $p=0.05$, black tea: 8% $p=0.04$, wood: 17% $p=0.02$), with a stronger response in lower quality substrates. To test the effects of temperature on the *ex-situ* soil respiration, we conducted two laboratory soil incubation experiments. In the first experiment, we derived microbial temperature response curves and calculated the Q_{10} in short-term incubations with temperatures ranging from 20°C to 60°C. In the second experiment, we fertilized soils incubated at 24°C and 28°C with six nutrient treatments to test if they constrained microbial respiration in warmed soils. Similar to previous studies, we found that sustained higher temperatures decreased the temperature sensitivity (Q_{10}) of the soils. We also found that microbial respiration in the warmed soils had the highest response to the C + Fertilizer treatment (respiration rate increased ~30% compared to the control treatment), showing that warmed soils were not just limited by labile carbon as expected, but also by other micro nutrients. These results suggest that warmer temperatures could: 1) with concomitant drying, slow carbon and nutrient turnover from lower quality litter to soil, and 2) drive increased soil microbial respiration until they are limited by labile carbon and micro nutrients, or until they eventually acclimate.

Poster #21-19**Title: Understanding Total Water Storage Anomalies Across the United States with Integrated Hydrologic Modeling and Satellite Estimates.**

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BER Program: SBR

Project: Interoperable Design of Extreme-scale Application Software (IDEAS)

Project Website: <https://ideas-productivity.org/ideas-classic/use-cases>

Modeling the global terrestrial water cycle has been referred to as the “grand challenge to hydrology”, which would enhance our understanding of scale-dependent relationships between subsurface and surface regimes, between land and atmosphere, and between human influence, including groundwater withdrawals, and future resources. Modern advancements in remote sensing have awarded scientists with the ability to measure mesoscale changes in Earth’s terrestrial water storage. The Gravity Recovery and Climate Experiment (GRACE) Program satellite observations measure fluctuations in Earth’s gravity attributable to mass flux, or changes in total water storage (TWS). However, GRACE TWS estimates are not without error and are limited in scale; GRACE uncertainty is still a topic of much discussion, and its products range in lateral resolution from 3° to 0.5°. Determining water resource availability for governance at the regional or major aquifer scale either involves downscaling coarse remote observations such as GRACE, or interpolating point observations (wells), both of which introduce uncertainty. Further, while we can infer from GRACE products the change in TWS from a baseline value, we do not know the total mass available, nor can we distinguish between processes driving mass change, such as recharge anomalies, natural variability or anthropogenic abstractions.

Here, I use an integrated hydrologic model, ParFlow, to support and better understand estimates of TWS from GRACE products in the continental United States (CONUS). The CONUS ParFlow configuration extends over a 6.3 million square kilometer area of the continental United States at 1-km lateral resolution. Previously, the CONUS model has been used to analyze continental-scale patterns of water table depth and its mechanistic relationship with topographic indices, recharge and evapotranspiration. This study seeks to use ParFlow to explain sources of groundwater storage loss or gain observed by GRACE remote sensing products. The CONUS model was run for water years 2009 through 2013 and compared to GRACE GFZ, JPL, and CSR gain-corrected time series. We identify regions in which ParFlow CONUS simulated storage change results fall inside GRACE leakage error, and we use ParFlow to explain partitioning of GRACE TWS into changes in snow water equivalent, soil moisture, groundwater, and surface water. ParFlow is also shown to be an effective tool for correcting signal attenuation in GRACE estimates. This study illustrates the benefit of extreme-scale hydrologic modeling, in that it helps bridge existing scale gaps between point observations and remote sensing and inform water resource governance at a range of scales.

Environmental System Science

Early Career Awards

Poster #1-37**Soil Carbon Storage and Loss Across a Tropical Forest Rainfall and Nutrient Gradients with Drying**

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Project: Early Career Award (Daniela Cusack)

Humid tropical forests contain some of the largest soil carbon (C) stocks on Earth, yet there is great uncertainty about how soil carbon dioxide (CO₂) fluxes will respond to projected changes in rainfall in this biome. Modeling experiments suggest that tropical forests will be more sensitive to changes in precipitation than to warming, opposite of trends in most other biomes. While shifts in soil moisture have been clearly linked to soil respiration, the magnitude of change in soil respiration may also be regulated by soil properties that influence root and/or microbial activity, like nutrient availability. To understand the potential effects of shifting rainfall on tropical forest soil CO₂ fluxes, we assessed seasonal patterns in soil respiration for 15 sites across rainfall and soil fertility gradients in Panama. We also established a 50% throughfall exclusion experiment at a subset of four sites. We predicted that changes in soil moisture would be the primary driver of soil respiration responses to seasonality, with a secondary role of nutrient availability in regulating the magnitude of the seasonal respiration response. We also predicted that the availability of organic C would be positively related to instantaneous soil CO₂ flux rates. We found that seasonal drying generally corresponded to declines in soil respiration, but there was great spatial variation, with a range of -19% to +360% in CO₂ fluxes during the wet versus dry season. The Wet:Dry season soil CO₂ flux ratio, used as an index of seasonal sensitivity, was best explained by a multiple regression including extractable resin P, base cations, and Wet:Dry season soil moisture ratios (positive relationships, $R^2 = 0.79$), with the strongest univariate relationship to resin-extractable P ($R^2 = 0.41$). Measures of dissolved organic matter were not related to soil CO₂ flux rates, but forest floor biomass accumulation during the dry season was positively related to soil respiration during the wet season ($R^2 = 0.26$), highlighting the contribution of litter decomposition to soil respiration. Preliminary results from the drying experiment indicate that instrumentation for soil temperature, moisture, CO₂ fluxes, and root productivity observation are all fully functional. Overall, our results from across the natural gradients indicate that scarce soil nutrients may be more important than shifts in soil moisture for driving seasonal soil respiration patterns across humid tropical forest landscapes. Thus, soil P and cation availability may determine tropical forest feedbacks to climatic change.

Poster #1-38**Topographic Controls over Greenhouse Gas Emissions from Puerto Rican Tropical Rainforest Soils**

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BER Program: TES

Project: Early Career Award (Melanie Mayes)

Project Website: <https://science.energy.gov/early-career/>

Humid tropical forests emit greenhouse gases including carbon dioxide (CO₂) and methane (CH₄) into the atmosphere, and a large proportion of these emissions are due to soil microbial respiration. Landscape position exerts key controls over emissions of CO₂ and CH₄, and the proportion of redox-active compounds like nitrate, sulfate, and iron in soils and soil water. I will present lab- and field-based measurements of soils from a 6-point valley to ridgetop transect in the Luquillo Experimental Forest in Puerto Rico, over the time frame before and after Hurricanes Irma and Maria. Surface soils were collected seasonally to determine basic soil characteristics, hydrolytic enzymes, and 16S ribosomal RNA gene sequencing. Soil water was collected following rainstorms using rhizon samplers at depths of 10 and 30 cm and analyzed for anions, cations, pH, and dissolved organic carbon and total dissolved nitrogen. Clear chloride and nitrate signatures are observed following the hurricanes, but to different extents depending on depth and landscape position. Soils were also incubated to quantify CO₂ and CH₄ emissions under oxic, anoxic, and fluctuating conditions. Finally, field-scale measurements of CO₂ and CH₄ were performed resulting in strong topographic gradients in gas emissions, e.g., valley soils emitted more CH₄. This poster will summarize key findings from a variety of observations with a focus on building a comprehensive understanding of differences as a function of topographic gradient, in order to build and test a model that considers both the geochemistry and microbiology of the soil environment.

Poster #21-34**Flux Chamber and Metagenomic Studies Provide Insights into Biogeochemical Mechanisms of Reactive Nitrogen Cycling in Soils of Mixed Hardwood Forests**

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BER Program: SBR

Project: Early Career Award (Jonathan Raff)

In terrestrial ecosystems, nitrogen (N) cycle processes play a crucial role in regulating the overall abundance of oxidized inorganic nitrogen and are responsible for initiating the subsequent loss of soil N via volatilization and leaching. Rates of nitrification and denitrification, pool sizes of nitrite and nitrate ($\text{NO}_2^- + \text{NO}_3^-$), and oxygen availability have been shown to be major determining factors in soil emissions of nitrogenous gases such as nitric oxide (NO) and nitrous oxide (N_2O). We investigated these factors in the context of two different mixed hardwood stand-types typically found throughout the Midwestern USA. Stand-type differentiation was based on whether plots were either dominated by trees that associate with arbuscular mycorrhizal fungi (AM) or ectomycorrhizal fungi (ECM). Metagenomic analyses revealed significant differences in the estimated copy numbers of N cycle genes, with AM soils possessing significantly greater copy numbers relative to ECM soil. Furthermore, the largest fluxes of N_2O and NO were observed under anaerobic conditions from AM soil. Additionally, AM soils possessed significantly larger pools of $\text{NO}_2^- + \text{NO}_3^-$ and more transcript copies of key nitrification and denitrification genes. We also find that when ECM soil is spiked with NO_2^- , N_2O production and denitrification transcript numbers rapidly increase. Together, these results indicate that anaerobic conditions in AM soil result in a significant loss of oxidized aqueous nitrogen via volatilization, and nitrogenous gas production in ECM soil is inherently limited by small pool sizes of $\text{NO}_2^- + \text{NO}_3^-$. At the ecosystem level, AM tree species have been encroaching rapidly into ECM-dominated forests throughout the Midwest (U.S.A). This change in tree species composition may significantly reorganize the soil microbial community leading to an increase the amount of nitrogen oxides being emitted from these ecosystems.

Poster #21-22**An Investigation of How Floodplain Deposit Ages and Permafrost Distributions Influence the Patterns, Rates, and Age of Soil Organic Carbon Fluxes to the Koyukuk River.**

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Project: Early Career

In the summer of 2018, we conducted a preliminary floodplain coring and river sampling program on the Koyukuk River and its associated floodplain in the vicinity of Huslia, AK. The Koyukuk River, one of the largest tributaries to the Yukon River, has one of the largest alluvial floodplains in Alaska. Scroll bar complexes, oxbow lakes, and peat-filled drained lake basin occupy the floodplain that reaches widths in excess of 15 km, creating a complicated mosaic of deposits that vary in age, permafrost extent, and soil organic carbon content. We mapped permafrost occurrence in exposed banks and soil cores. We observed that the presence and absence of permafrost extent in the floodplain ranged at scale of kilometers, in scroll bar complexes of varying age, to tens of meters along individual scroll bars. Analysis of aerial photographs and high-resolution satellite imagery allow us to quantify bank erosion rates at decadal and yearly time scales along 10s of km of the river at 2 m spatial resolutions. Comparing these erosion rates and patterns to our permafrost mapping allows us to explore whether, and at what scales, the presence of permafrost controls river bank erosion rates. We analyzed soil samples from cores and river bank exposure for carbon content, grain size, and radio carbon ages. This data will allow us to develop an estimate of the floodplain carbon storage and age of deposits. A comparison of the age distribution of floodplain material eroding into the river to dissolved organic carbon (DOC) radio carbon ages of river water will allow us to begin to explore the influence of bank erosion on the composition of river carbon fluxes.

Poster #1-39**Improved Representations of Methane Emissions from Wet Tropical Forest Soils using a Microbial Functional Group-Based Model**

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BER Program: TES

Project: Early Career Award (Melanie Mayes)

Project Website: <https://science.energy.gov/early-career/>

Tropical ecosystems contribute significantly to global emissions of methane (CH₄). However, landscape topography largely controls the rate of CH₄ emissions from wet tropical forest soils. Here we attempt to explain the dynamics of CH₄ emissions from two growing seasons (2015 and 2016) across a ridge-slope-valley topographic gradient in the El Yunque National Forest, Puerto Rico using a microbial functional group-based model. In 2016, CH₄ emissions follow the trend of valley>>slope>=ridge, which is different from the observed dynamics of CH₄ emissions during a drought and follow-up wet-up event in 2015. Soil temperature ranges were overlapping across topographic locations for both years. In contrast, soil water (and oxygen) ranges, as well as porewater chemistry (pH and organic acids) were different for the ridge vs. valley soils and were different between drought and non-drought years. These changes are expected to alter the substrate for CH₄ production and CH₄ consumption as well as the dynamics of respective microbial functional groups (acetotrophic or hydrogenotrophic methanogens and methanotrophs), which in turn, can influence net emissions of CH₄. Thus, contrasting patterns of soil water (and oxygen) and associated soil biogeochemistry between ridge vs. valley soils played an instrumental role in CH₄ emissions from the wet tropical soil of Puerto Rico, which were reproduced by a microbial functional group-based model. A variance-based sensitivity analysis further suggested that parameters related to acetotrophic methanogenesis and methanotrophy were critical for simulation of net CH₄ emissions across the topographic locations. To conclude, this study contributes to the ongoing development and improvements of the Earth system models to better simulate the microbial roles on methane cycling at regional and global scales.

Poster #1-40**Tropical Forest Response to a Drier Future: Synthesis and Modeling of Soil Carbon Stocks and Age**

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BER Program: TES

Project: Early Career Award (Karis McFarlane)

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 are compiling carbon and radiocarbon (¹⁴C) soil profile data from the tropics including sites in Mexico, Brazil, Costa Rica, Puerto Rico, Peru, Cameroon, and Indonesia. Our sites represent a large range of moisture, spanning 710 to 4200 mm of mean annual precipitation, and include Andisols, Oxisols, Inceptisols, and Ultisols. We compared measured soil C stocks and ¹⁴C profiles to data generated from CLM and ELM. 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. We found that modeled carbon stocks were consistently higher than measured stocks, modeled soil carbon ages were older than measured values near the surface (upper 50 cm), and that modeled soil carbon ages for deep soil carbon were younger than measured deep soil carbon ages. Finer resolution runs of ELM-ECA and CTC 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 and litterfall) in driving vertically-resolved measured and modeled soil carbon pools and ages.

Poster #1-41**Soil Radiocarbon Measurements Across Climatic, Edaphic, and Physiographic Gradients in Tropical Forests**

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BER Program: TES

Project: Early Career Award (Karis McFarlane)

Tropical forests account for 29% of global soil carbon, but much of this belowground carbon is stored in pools with short (decadal) turnover times with a potential for rapid response to future change. Moisture may be more important than temperature in driving soil C storage and emissions in the tropics, yet the role of moisture on soil C dynamics is understudied and underrepresented in land surface models. We measured or attained data for soil carbon stocks and radiocarbon (¹⁴C) values of profiles from the tropics including sites in Puerto Rico, Mexico, Costa Rica, Panama, Brazil, Peru, Cameroon, and Indonesia. 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. Collaborative site-specific studies to explore the influence of controlling factors in manipulation experiments and constrained gradients of precipitation, soil type, root inputs, geomorphology, and landuse on carbon storage and turnover soil characteristics, root inputs, topography 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 to secondary forests restored young soil C stocks after 15 years, but young secondary forests retain a legacy of lost carbon. Site-level runs of ELM v.1 and integration with a reduced complexity model (SoilR) will be used to evaluate model representation of soil C processes, including vertically-resolved carbon transfer rates, root inputs, and decomposition.

Terrestrial Ecosystem Science

University Awards

Poster #9-33**Quantitative, Trait-Based Microbial Ecology to Accurately Model the Impacts of N Deposition on Soil C Cycling in the Anthropocene**Edward Brzostek^{1*}, Ember Morrissey¹, Zachary Freedman¹, Steve Blazewicz², and Peter Weber²¹ West Virginia University, Morgantown, WV;² Lawrence Livermore National Laboratory, Livermore, CAContact: rbrzostek@mail.wvu.edu

BER Program: TES

Project: University Award

Atmospheric nitrogen (N) deposition resulting from fossil fuel burning in the eastern United States has altered fundamental soil processes, challenging our understanding of whether soils will continue to sequester carbon (C) from the atmosphere and slow environmental change. While evidence shows that N deposition has enhanced C storage in temperate forest soils, it remains unclear whether these effects will persist. Moreover, there is uncertainty as to why some forest soils gain more C in response to N deposition than others. At the heart of this knowledge gap is a failure to link N-induced shifts in microbial biodiversity with their 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 shifts in key microbial traits drive soil C stabilization following N deposition.

Microbial growth, C use, and N use efficiency (the ratio of C or N used to produce microbial biomass vs. the total C or N that a microbes takes up) and turnover (microbial death rate) are keystone microbial traits that control soil processes. Microbes need N as a nutrient to grow, and N deposition could shifts these traits. For example, if high N levels increase C use efficiency and turnover, there will be greater production of dead microbes, which stick to charged soil mineral surfaces and are protected from further microbial attack. To date, there remain limited data on how these traits vary across environmental gradients. Moreover, these N deposition impacts on soil C may likely vary across tree species that differ in the type of symbiotic fungi their roots support: arbuscular mycorrhizal (AM) fungi or ectomycorrhizal (ECM) fungi. AM forests have easier to break down dead plant material, greater bacterial dominance, and more soil N than ECM forests, which could explain why forests differ in soil C responses to elevated N.

The uncertainty highlighted above is mirrored in models used to predict future soil C stocks because they are sensitive to estimates of microbial traits. As measures of microbial traits are sparse, most models assume these traits are the same across environmental gradients, which impedes our ability to predict future soil C stocks. Thus, our objectives are to 1) Quantify variation in taxon-specific and community-level microbial traits across gradients in microbial community composition, mycorrhizal symbioses, and N availability and 2) Integrate this data into a novel predictive framework that enhances our ability to project the regional soil C consequences of historical N deposition in temperate forests.

To meet our objectives, we will link data generated by our novel quantitative stable isotope probing methodology for measuring taxon-specific traits with a state-of-the-art microbial decomposition model. We will measure microbial traits and diversity across three Eastern temperate forest sites of the National Ecological Observatory Network in MA, VA, and TN that span a historical N deposition gradient. At each site, we will use six forest plots dominated by either ECM or AM associated trees thereby leveraging an additional axis of variation in litter quality, soil chemistry, and microbial biodiversity. To isolate N effects, we will incorporate an existing N fertilization experiment in WV. The data we generate will flow into transforming a model that predicts differences between AM and ECM forests in soil C processes.

Poster #9-43**Space-Based Estimates of Amazon Basin GPP Using Atmospheric Carbonyl Sulfide**

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BER Program: TES

Project: University Award

Terrestrial photosynthesis is the fundamental coupling between global cycles of energy, carbon, and water (Figure 1). Photosynthesis is driven by incoming radiation and water availability, modulates atmospheric carbon and in turn releases water vapor that can drive cloud distributions and rainfall. But the most productive region on Earth, the tropical biosphere, remains a critical blind spot in our attempts to understand photosynthesis. Even groundbreaking satellite observations of solar-induced chlorophyll fluorescence (SIF) are largely obscured by the persistence of tropical clouds. What lies beneath these clouds is the central enigma of the carbon cycle.

Here we leverage the temporally and spatially integrative attributes of atmospheric carbonyl sulfide (OCS or COS) to fill the critical gaps left from other regional analysis, creating a necessary and complementary measurement. The atmospheric OCS tracer is related to a temporally and spatially integrated measurement of photosynthesis that is upwind of the OCS measurement. When clouds are present, the ability to accurately measure OCS is lost. However, the photosynthesis signal is preserved in time as the accumulated atmospheric OCS signal. When the clouds clear or when the air parcel is transported by wind and convection away from the clouds, the subsequent atmospheric OCS measurement provides an integral view of the photosynthesis fluxes that were upwind of where the OCS measurement was made. Thus, the atmospheric OCS variation provides an archive of the photosynthesis activity that can be collected by satellites at times and locations that are not contaminated by clouds. This unique temporal integration of the OCS method could have a transformative effect on our ability to uncover the mysteries of photosynthesis in the tropics.

We inferred regional GPP estimates from space-based observations of upper tropospheric atmospheric OCS (Figure 1). The analysis was based on global atmospheric chemical transport simulations (GEOSCHEM) that were linked to global ecosystem flux estimates (SiB). The OCS satellite constraint on these simulations resulted in a measurement-based estimates of Amazon basin-wide GPP that overlaps with the range of GPP estimates reported in previous bottom-up and ecosystem modeling studies, building confidence in this new independent tracer technique.

Poster #9-32**Sticky Roots--Implications of Widespread Viral Infection of Plants for Soil Carbon Processing in the Rhizosphere**

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BER Program: TES

Project: University Award

One way that plants strongly influence soil properties is through rhizodeposition, in which exudates diffuse from roots, additional secretions are actively released, and root cells are sloughed into the soil. The core objective of this project is to test whether rhizodeposition can destabilize soil organic matter (SOM) association with minerals, making that SOM more vulnerable to microbial attack.

Mineral associations preserve very large soil carbon pools in terrestrial ecosystems, and DOE's newly developed E3SM Land Model (ELM) includes a representation of that soil carbon preservation. However, the potential vulnerability of SOM–mineral associations to effects of rhizodeposition is not yet represented in ELM. In a novel approach, we are exploring whether plant virus infection can serve as a tool to intensify rhizodeposition, and therefore intensify dissolution of SOM from minerals. Viral infection is widespread in terrestrial ecosystems; 25- 70% of plants have virus infection, yet the influence of such infection on root traits and terrestrial soil carbon dynamics remains largely unexplored.

We are using two plant hosts--the annual *Avena sativa* (oats) and the genetically tractable, model grass *Brachypodium distachyon*—and the broad host range virus Barley Yellow Dwarf Virus (BYDV). BYDV infects at least 150 grass species in agricultural and natural ecosystems, and in previous experiments, roots of oats infected with BYDV had extraordinarily sticky roots, suggesting that infection enhanced rhizodeposition. Uninfected and infected individuals of each host species are being grown individually in replicate "rhizoboxes" (rectangular pots equipped with sensors) for: (1) sampling of organic compounds inside phloem before they diffuse out to soil (using aphid stylectomy); (2) biogeochemical profiling around roots (using Eh and pH sensors, and, sampling of dissolved organic compounds in soil solution); (3) imaging of regions around root supporting extensive microbial growth using living, luminescent microbial biosensors; and (4) incubation and subsequent quantification of mineral- SOM associations in the presence of uninfected vs. infected plant roots. Mechanistic understanding derived from these data will inform future development and application of ELM. If our experiments indicate that high rates of rhizodeposition support a large, active microbial population driving SOM-mineral dissociation, then future research combining experimentation and modeling should explore the strength and larger-scale significance of that cascade of processes. And if viral infection does lead to "sticky roots", our understanding of the potential importance of prevalent virus infection in terrestrial landscapes will be transformed.

Poster #9-25**Resolving Conflicting Physical and Biochemical Feedbacks to Climate in Response to Long-Term Warming**

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Project: University Award

Microorganisms regulate soil carbon (C) cycling, and several mechanisms mediate the warming effects on microbial physiology and climate feedbacks to the atmosphere. Microbial growth strategy, substrate complexity, and physical protection all contribute to microbial C processing and soil organic matter loss or stabilization. In a 27-year experiment at Harvard Forest, soils have been continuously heated 5°C above ambient temperatures, with unheated plots as controls. Chronic warming reduced microbial C-use efficiency and mass-specific growth, while warming increased turnover rate in microaggregates (<250 µm) and macroaggregates (250-2000 µm) extracted from the top 10 cm of the mineral soil. Microbial efficiency declined with substrate complexity, consistent with previous results. C-use efficiency was more temperature sensitive in warmed soils, in microaggregates compared to macroaggregates, and with complex substrates. Warmed soil aggregates had reduced C and nitrogen content, enzyme production, and increased the proportion of mineral-associated organic matter. Structural equation modeling showed that soil warming regulated growth efficiency directly and indirectly by altering soil structure, substrate availability, and microbial physiology. Scanning Transmission X-ray Microscopy and X-ray Raman Scattering results show that physically protected C inside soil aggregates is not as weathered as inter-aggregate C budget. Analyses done with the trait-based model MIMICS (Microbial-Mineral Carbon Stabilization Model) suggest that long-term warming effects of soil C more closely resemble observed values when physical protection of soil organic matter is a function of microbial biomass and clay content, compared to clay content alone. Our findings show essential roles of the mechanism-related factors in mediating microbial thermal strategy and physiology in response to climate warming, suggesting the need to include these mechanisms in earth system models to improve predictions of soil C feedbacks to the climate system.

Poster #9-18**Peatland Hydrology Across Scales: Coupling Carbon Emissions with Water Table Fluctuations**

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BER Program: TES

Project: University Award

Our project aims to guide future representations of peatland hydrology and water-carbon feedbacks within Earth System Models, by developing a nested series of parsimonious, stochastic, and process-based hydrological models that can quantify the effects of temporal hydroclimatic variability and spatial heterogeneity on peatland carbon emissions. Due to the influence of water table depth on aerobic versus anaerobic conditions, which control the oxidation and production of CH₄ within the peat column, water table fluctuations can strongly regulate the timing and magnitude of these metabolic processes. Thus, our research questions are centered on the three key drivers of water table fluctuations within peatland watersheds: (1) temporal hydroclimatic fluctuations, (2) spatial heterogeneity of bog microtopography, and (3) hydrological connectivity across the peatland watershed. We intend to validate our models against existing long-term datasets within the Marcell Experimental Forest (MEF), and collect new data whenever necessary.

To date, we have installed automated water table gauges (in summer 2018) at the bog-forest boundary at MEF, which will give us new information about the timing and amount of lateral water subsidies into the bog from its surrounding upland forests. These lateral inputs are expected to magnify the hydrological response within the bog during high intensity rainfall and snowmelt events. Furthermore, we have demonstrated using eddy covariance data at MEF that the annual CH₄ emissions is strongly correlated with later onset of seasonal infiltration (i.e., if snowmelt and heavy precipitation occur later in the year). Currently, we are working to incorporate the seasonal dynamics of specific yield, lateral flow, and precipitation into a water balance model that will be used to predict the daily and seasonal variations in water table depths. This water balance model will be coupled to a new, stochastic reaction kinetics model to predict peatland carbon emissions in response to variable hydroclimatic forcing.

Poster #9-34**Carbon–Nutrient Economy of the Rhizosphere: Improving Biogeochemical Prediction and Scaling Feedbacks from Ecosystem to Regional Scales**

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Project: University Award

We advance plant-soil-microbial dynamics in terrestrial biosphere/Earth system models in three areas: i) nutrient cycling and plant uptake (nitrogen and phosphorus); ii) root exudation and priming; and, iii) mycorrhizal dynamics. We leverage a multi-site mycorrhizal gradient across the US to update the Fixation & Uptake of Nitrogen (FUN) submodel embedded within CLM 5.0. FUN-CLM specifies the site data collection, which includes soil, leaf chemistry, and litterfall sampling from multiple plots at each site. A remote sensing component expands the observational constraints to the model globally.

Site results show that ECM plots are more nutrient limited than are AM or mixed plots. ECM plots have lower soil pH, higher soil C:N, higher leaf litter lignin:N, and lower microbial growth efficiency than AM plots, the latter likely reflecting the necessity for greater enzyme investment by ECM soil microbes to degrade soil organic matter; this is supported by higher rates of lignolytic enzymes activity. Long-term experiments are monitored with minirhizotron tubes, root ingrowth cores, and ¹³C isotopically distinct soil cores for belowground inputs.

Concurrently, we developed the C cost of P uptake computational framework in FUN, as well as the additional C and N cost of synthesizing phosphatase enzymes to extract P from soil (FUN-P). The model is currently parameterized with the site data and previous data at a subset of the sites, resulting in differences in costs, uptake, and nutrient cycling between ECM and AM trees in the model. FUN-P accurately estimates measurements of P retranslocation across sites. The inclusion of costs for P uptake improves the ability of the model to capture observed patterns in C allocation to root exudation and mycorrhizal biomass. Collectively, the modeling activity provides a novel framework for understanding how interactions between the C-N-P cycles belowground impact the ability of plants to acquire nutrients and support NPP. We are currently working to couple FUN-P to CLM and to ELM/E3SM.

Finally, we are developing a remote sensing analysis of mycorrhizal association, extending previous work done at 4 sites across 150K trees to the global scale across over 100K plots encompassing millions of trees. This will create the first ever, global, spatially explicit, 30 m resolution, observational dataset of mycorrhizal association. These data will provide a major breakthrough not only in understanding ecosystem carbon-nutrients exchange and links between belowground and aboveground processes, but will also be directly used to initialize and constrain the global modeling developments described above.

Poster #1-30**Shrub Expansion Alters Root Traits in the Arctic**

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BER Program: TES

Project: University Award

Deciduous shrub encroachment is occurring across the arctic tundra. Increases in shrub cover could alter belowground carbon and nutrient dynamics as a consequence of shifts in root function. However, root dynamics associated with shrub expansion remain one of the least understood aspects of plant function in the Arctic. We sampled roots of common deciduous shrub genera (*Betula*, *Alnus*, and *Salix*) and tussock grass/sedge vegetation (dominantly *Eriophorum* spp.) in five moist acidic tundra sites along a latitudinal gradient in Northern Alaska (67.0 °N – 69.3 °N). Root morphology and mycorrhizal colonization of the non-woody absorptive roots were measured for both shrubs and tussock vegetation. Vertical distributions of absorptive root biomass within a shrub or tussock patch (1-m diameter) were determined from soil coring to the bottom of the active layer.

We found changes in root traits consistent with higher nutrient demand of shrubs. Shrubs had thinner roots than grass/sedge species at all the five sites, and shrub roots were frequently colonized by ectomycorrhizal fungi whereas tussock roots were non-mycorrhizal and rarely branched. The active layer was deeper in shrub patches than tussock patches at the two northern (colder) sites, and there were substantial roots below 20cm under the shrub patches. These findings suggest deeper rooting and higher capacity for resource acquisition associated with shrub expansion in Northern Alaska. Such changes may accelerate nutrient cycling and potentially stimulate carbon mineralization in both surface and deep soils, and a possible positive feedback to Arctic warming. We also found pronounced differences in root traits among shrub genera. *Salix* had absorptive roots that were generally thinner and less dependent on ectomycorrhizal fungi than *Betula* and *Alnus*. The accumulative root biomass in the active layer was higher under *Alnus* patches than *Betula* patches at the southernmost site. In contrast, *Betula* patches had the most abundant roots at the two northern sites, especially in the deeper layers. These climate-dependent variations indicate that deciduous shrub genera employ unique root strategies despite their similar growth form. The consideration of tundra root-trait data across an environmental gradient may enhance our ability to forecast how climate change will affect belowground functioning in the Arctic.

Poster #9-19**How do Whole-Ecosystem Warming and Elevated Atmospheric Carbon Dioxide Concentrations Affect Peatland Methane Production**

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BER Program: TES

Project: University Award

Peatlands contain one-third of the world's soil carbon (C). Much of this C is stored deep in the soil profile, where water-logged and anaerobic conditions have allowed C to accumulate for thousands of years. It is currently unknown if these vast C stores will remain belowground or if they will be respired as carbon dioxide (CO₂) and/or methane (CH₄) in the face of ongoing global change. Understanding, and modeling, the future fate of this soil C remains a pressing issue in global biogeochemistry. We assessed the response of CO₂ and CH₄ production in a boreal peatland following 13 months of deep-peat warming (DPW), 16 months of subsequent whole- ecosystem warming (surface and deep warming; WEW), and 4 months of elevated atmospheric CO₂ concentrations as part of the Spruce and Peatland Responses Under Changing Environments (SPRUCE) project in northern Minnesota, USA. This project includes 5 temperature treatments that warmed the entire 2 m peat profile from 0 to +9 °C above ambient temperature with and without elevated atmospheric CO₂ concentrations (~850 ppm). Soil cores were collected at multiple depths beneath the peatland surface (-20 to -200 cm) from each experimental enclosure at SPRUCE and anaerobically incubated at in situ temperatures for 1-2 weeks. Following DPW, only CH₄ production from surface depths (e.g., -30 cm) was positively correlated with elevated temperature. However, during WEW, both surface and deep peat CH₄ production increased with rising temperature. There was little indication that elevated CO₂ influenced CH₄ production. Surface peat had greater CH₄ production than deeper peat, implying that increased CH₄ emissions in response to warming observed in the field were largely driven by surface peat dynamics. Radiocarbon analyses suggest that CO₂ and CH₄ are produced from the decomposition of both young and ancient C sources. The CO₂:CH₄ ratio was inversely correlated with temperature across all depths during WEW, indicating that the entire peat profile is becoming more methanogenic with warming. This result was supported by *in situ* measurements of porewater CO₂ and CH₄ concentrations which displayed the same trend. Thus, our results suggest that the vast C stores at depth in peatlands are responsive to warming only after a significant lag period, but that ecosystem responses remain largely driven by surface peat.

Poster #9-20**Whole Ecosystem Warming Stimulates Greenhouse Gas Production and the Mobilization of Ancient Peat Carbon in Northern Peatlands**

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BER Program: TES

Project: University Award

The goals of this research are to investigate the metabolic pathways of soil organic matter decomposition, controls of greenhouse (GHG) production, and the response of the microbial C cycle to environmental change (warming, CO₂ enrichment). Multiple field campaigns were conducted to capture the response of whole-ecosystem warming (WEW) at the Marcell Experimental Forest (MEF), Minnesota, where the Oak Ridge National Lab (ORNL) has established the Spruce and Peatland Response Under Changing Environments (SPRUCE) experiment. Greenhouse gases (CO₂, CH₄), the environmental metabolome, and microbial communities were characterized using advanced analytical chemistry and environmental genomics techniques. Four years after initiation of deep peat heating, multiple lines of evidence indicate that WEW stimulates organic matter decomposition and leads to substantial alteration in the belowground carbon cycle. While we observe increases in both CO₂ and CH₄ production, CH₄ shows a greater response to temperature as evidenced by declining CO₂:CH₄ ratios in the shallow subsurface (<30cm). To further inform this shift towards increasing methanogenesis, we examined changes in microbial genomic traits, metabolites, and proteins involved in organic matter degradation. Concomitant with increases in CH₄ production, we observe increases in the relative abundance of hydrogenotrophic methanogens along with microbial enzymes diagnostic of methanogenesis. Sugars and fermentation products were positively correlated with increasing temperature in heated treatments relative to controls. Thus, it appears that warmer temperatures stimulate photosynthetic production, thereby releasing labile C (e.g. sugars) from plants which, in turn, stimulates fermentation increasing the availability of substrates that ultimately lead to increasing surficial methane production with warming. Results from microbial community analysis also show an increase in the relative abundance methanotrophic bacteria and an overall decline in microbial diversity with WEW. While the response of the shallow subsurface peat to warming appears to be strongly affected by fresh plant inputs, in deeper peat (>30 cm), we observe radiocarbon (¹⁴C) evidence for the release of old catotelm carbon in response to warming. Four years from the onset of deep peat heating, the respiration product, dissolved inorganic carbon (DIC), is ¹⁴C-depleted in the +9°C treatment plot in comparison to similar depths in the control plots up to 2m deep in the peat. These results suggest that ancient catotelm C is mobilized and respired in the heated treatments. Further analyses will reveal whether this mobilization of ancient C is solely the result of warming or may be stimulated by downward advection of increasing labile C inputs from the surface (i.e. priming).

Poster #9-26**Building Coastal Models with the Salt Marsh Accretion Response to Temperature eXperiment (SMARTX)**

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BER Program: TES

Project: University Award

The Energy Exascale Earth System Model (E3SM) simulates fully coupled processes and interactions between water, energy, carbon and nutrient cycles. E3SM connects vegetation and soil dynamics through nutrient uptake, plant production, litterfall and decomposition as a function of abiotic parameters (i.e. temperature and moisture). However, E3SM is designed to characterize terrestrial and freshwater habitats and connects terrestrial and open ocean ecosystems using a single transport term, ignoring coastal dynamics. The goals of our project were to: 1) Parameterize a point version of E3SM to mimic coastal wetland habitats and 2) Determine C₃ and C₄ marsh community responses to the interacting effects of sea level rise, increased temperature, and elevated CO₂ (eCO₂) demonstrated in the Salt Marsh Accretion Response to Temperature eXperiment (SMARTX). We adapted E3SM to a coastal ecosystem using long-term data sets from field experiments conducted at the Global Change Research Wetland (GCRew). Tidal forcing was mimicked using a 2-column system. Column 1 simulated interactions between vegetation and soil while column 2 simulated water level (both tidal and sea level rise). Parameters for generic C₃ and C₄ plant functional types were adapted to represent saltmarsh C₃ and C₄ communities. We also altered biogeochemical processes to incorporate salinity, methane, and sulfur dynamics.

Plant community responses to environmental change were non-linear, non-additive and inconsistent between C₃ and C₄ plants. We were able to characterize the following shifts observed in SMARTX results: alterations to above:below ground biomass ratios with eCO₂ in C₃, but not C₄ communities; peak biomass responses to moderate temperature rise and decline with further warming; synergistic effects of warming and eCO₂ on biomass allocation in C₃ communities.

Poster #9-31**Using Root and Soil Traits to Forecast Woody Encroachment Dynamics in Mesic Grassland**

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BER Program: TES

Project University Award

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 changes in drought intensity and woody encroachment - a process that results in increased woody plant abundance corresponding with decreased herbaceous plant abundance. The combination of reduced soil moisture and shifts in plant dominance from herbaceous to woody are likely to alter C pools in the soil profile. In order to predict changes in grassland vegetation structure and the associated impacts on C cycling requires greater understanding of changes in soil C pools at multiple soil depths, and the responses of these pools to changes in precipitation. The Land Surface Model (LSM) component of Earth System Models has the ability to capture these dynamic changes in ecosystem function, but lack the data to accurately parameterize these processes at multiple depths within the soil profile.

We have developed a set of objectives that combine observational, experimental and modeling approaches to improve our ability to project ecosystem consequences of shrub encroachment in the US Great Plains region. We propose 3 main objectives: (1) Quantify differences in aboveground (stem and leaf biomass) and belowground C pools (root C, microbial C, bulk soil C) using detailed excavations of entire mixed shrub-grass assemblages. We will subsample portions of the rhizosphere for detailed root physiological and microbial activity measurements; (2) Using rainout shelters built over mature shrub-grass communities, we will experimentally reduce the amount of precipitation. Comparing responses among shrubs and grasses, we will measure differences in source-water use, above and belowground productivity, canopy water stress, soil and microbial C and microbial C-cycling activity, and changes in plant cover and community dynamics; (3) Using a global demographic LSM (CLM FATES), we will forecast the impacts of available water on shrub-grass cover in the central Great Plains region, and the resulting effects of these dynamics on ecosystem services (aboveground production, above- and belowground C budgets). The experiment-modeling framework described here will improve our understanding of interactions and feedbacks between aboveground and belowground processes, by specifically measuring plant-soil-microbial traits at various depths in the soil profile. The details of these coupled interactions will improve the representation of subsurface processes in LSMs and will improve forecasts of dynamic changes in ecosystem structure in grassland ecosystems.

Poster #1-67**Extrapolating Ecosystem Processes of Seasonally Dry Tropical Forests Across Geographic Scales and into Future Climates**

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Project: University Award

Seasonally dry tropical forests (SDTFs) experience a pronounced dry season lasting 3 to 7 months and were once abundant. Dry forests are understudied compared to tropical rain forests, and are poorly represented in earth system models. Important knowledge gaps include: i) whether SDTF are vulnerable or resistant to changing rainfall regimes, ii) which nutrients, if any limit ecosystem processes, and iii) how nutrients and water interact to shape forest structure and function. We addressed these questions using multiple approaches including long-term observations, ecosystem-scale experiments, vegetation modeling, and surveys of plant hydraulic traits and allometry. Our results are transforming our understanding of this biome. First, the long-term records of forest mortality to show that a SDTF in Costa Rica is extremely sensitive to extreme drought, and that hydraulic safety margin explains interspecific variation in tree mortality. Second, the factorial nitrogen x phosphorus fertilization experiment showed that phosphorus addition increases fine root production, presumably because after phosphorus limitation is alleviated, trees become limited by water. Third, our large-scale throughfall exclusion x nutrient addition experiment confirms that nutrients and water interact to regulate productivity, but effects depend upon tree species. Last, our measurements of plant hydraulic traits in Colombia, Costa Rica, Mexico, and Puerto Rico underscore how rainfall regimes shape ecosystem function.

We have developed models to complement our empirical work. (i) Hydraulic traits have been implemented into ED2, and have been shown to be essential for simulating tropical dry forest phenology. Given our mortality observations, these hydraulic traits are also essential for the development of an improved mortality parameterization. (ii) In order to better understand the role of nutrients in this biome, we coupled for the first time a vegetation demographic model (ED2), a model microbial dynamics with carbon-nitrogen-phosphorus biogeochemistry (MEND), and a mechanistic model for nutrient competition (N-COM). This work illustrates how observed variation in soil properties can drive large variation in forest functioning and composition during secondary forest succession. (iii) We have also used this model to better understand the results from our nutrient fertilization experiment. As in the observations, the model simulates an increase in fine root production following phosphorus addition. The reason is that P addition makes the ecosystem more water limited, and the model responds by facultatively increasing the amount of fine roots per plant. Collectively, our results underscore how water and nutrients interact in fundamentally different ways in tropical dry compared to rain forests.

Poster #1-31**Changing Characteristics of Runoff and Freshwater Export From Watersheds Draining Northern Alaska**

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BER Program: TES

Project: University Award

The quantity and quality of river discharge in arctic regions is influenced by many processes including climate, watershed attributes and, increasingly, hydrological cycle intensification and permafrost thaw. We used a hydrological model to quantify baseline conditions and investigate the changing character of hydrological elements for Arctic watersheds between Point Barrow and just west of Mackenzie River over the period 1981-2010. The region annually exports 28.1 km³ yr⁻¹ of freshwater via river discharge, with 51.9% (14.6 km³ yr⁻¹) coming collectively from the Colville, Kuparuk, and Sagavanirktok rivers. Our results point to significant ($p < 0.05$) increases (134-212% of average) in cold season discharge for several large North Slope rivers including the Colville and Kuparuk, and for the region as a whole. A significant increase in the proportion of subsurface runoff to total runoff is noted for the region and 24 of 42 study basins, with the change most prevalent across the northern foothills of the Brooks Range. Relatively large increases in simulated active-layer thickness suggest a physical connection between warming climate, permafrost degradation, and increasing subsurface flow to streams and rivers. A decline in terrestrial water storage is attributed to losses in soil ice that outweigh gains in soil liquid water storage. Over the 30 yr period the timing of peak spring (freshet) discharge shifts earlier by 4.5 days, though the time trend is only marginally ($p = 0.1$) significant. These changing characteristics of Arctic rivers have important implications for water, carbon, and nutrient cycling in coastal environments.

Poster #9-27**Modeling Tidal Marsh Carbon Cycling Under Sea Level Rise and Elevated CO₂**

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Project: University Award

Coastal marsh, mangrove, and seagrass ecosystems are of global importance in terms of carbon cycling despite occupying just 2.5% of worldwide land area. These systems account for almost half of total marine carbon burial and sequester carbon at extremely high rates, thus we must work towards predicting the dynamic responses of coastal carbon pools to shifts in climate and rising sea levels. Complex interactions between the biotic and abiotic constituents of coastal ecosystems shape carbon cycling processes, but modeling efforts to date have not fully captured the feedbacks that control carbon burial and organic matter accumulation under global change scenarios over decades to centuries. We present a new point-based soil cohort model that captures the ecogeomorphic feedbacks between flooding, organic matter accumulation, sediment deposition, and marsh surface elevation under scenarios of accelerated sea level rise and elevated CO₂. Our model incorporates the differential effects of inundation and resource supply on primary production of two coastal plant types (C3 & C4), and couples this with organic matter decomposition in the soil as a function of age, carbon quality, depth, and carbon priming by roots. This allows us to predict dynamic changes in surface elevation and carbon burial over annual to decadal time scales, and to predict how accelerating sea level rise rates and alterations in mineral sediment supply will alter these feedbacks over decadal to centurial time scales. Preliminary results indicate that coastal marsh elevation can reach an equilibrium with rising sea levels via organic accretion even with limited mineral sediment inputs, and that elevated levels of atmospheric CO₂ can further enhance carbon sequestration and subsurface organic accretionary processes through effects on belowground primary production. However, under scenarios of accelerated sea level rise, the model indicates a point at which the reduction in primary production is not compensated by increased mineral deposition, leading to the drowning of the marsh. Our work highlights the importance of organic accretion in future marsh survival.

Poster #1-32**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 Award

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New estimates place 1460-1600 billion tons of soil carbon in the northern circumpolar permafrost zone, more than twice as much carbon than in the atmosphere. Understanding the magnitude, rate, and form of greenhouse gas release to the atmosphere is crucial for predicting the strength and timing of this carbon cycle feedback to a warming climate. Here we report results from an ecosystem warming manipulation where we increased air and soil temperature, and degraded the surface permafrost. We used snow fences coupled with spring snow removal to increase deep soil temperatures and thaw depth (soil warming) and open top chambers to increase growing season air temperatures (air warming). The soil warming treatment has successfully warmed soils by 2-3°C 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. We have subsequently manipulated the surface water table that together with warming influences air and deep soil temperatures, permafrost, and soil moisture conditions that are primary drivers of tundra ecosystem carbon balance across the Arctic landscape. Here we report measurements of long-term carbon dioxide and methane exchange as a metric of changes in ecosystem carbon storage. Overall, soil warming had a much stronger effect than air warming, and the dynamics changed non-linearly over the course of the long-term experiment. Soil warming that degraded permafrost stimulated both gross primary productivity (GPP) and ecosystem respiration (ER) such that the system was initially a net sink of C in the growing season. In the second phase (6-10 years), ground subsidence as a result of thaw continued to increase soil moisture and saturate the soil. While permafrost thaw continued to progress, both GPP and ER became suppressed and resulted initially in neutral growing season C exchange, and eventually net C release (source). Soil warming has also altered the form of C release, as measurements have now documented a 3-20x increase in CH₄ emissions depending on how wet the soil became after permafrost degradation. The negative responses of plants and soils to continued permafrost thaw were not simulated by the CLM model, which projected increased GPP and ER with increased thaw. This suggests improved model structure that includes the physical subsidence of ground, which causes surface soils to become wetter, may be needed in order to capture the non-linear dynamics revealed by this unique long-term experiment.

Poster #9-28**Wood Decomposition: Understanding Processes Regulating Carbon Transfer to Soil Carbon Pools Using FACE Wood at Multiple Scales**

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Project: University Award

Dead wood is a significant terrestrial carbon (C) pool, comprising approximately 20% of the forest biomass in the U.S. A major uncertainty in the terrestrial C cycle is the transfer of C from that dead wood into the underlying mineral soil C pool, where it may be incorporated into recalcitrant or protected soil C pools during the decomposition process. Documenting the fate of wood C during the decomposition process is difficult because (1) wood decomposition is inherently slow, (2) C from decomposing wood often cannot be differentiated from C in the soil matrix, and (3) microbial decomposers with distinct mechanisms can drive distinct outcomes, poorly predicted by climate alone. While Specific wood-decay fungi (brown rot & white rot) and invertebrates, especially termites, are understood to be the principal agents mediating wood decay, little is known about their ecology or their interactions, nor the process and pathways affecting the transfer of wood to the soil.

The FACE Wood Decomposition Experiment (FWDE) was established in 2011 with wood grown under the elevated CO₂ in the free-air carbon dioxide enrichment (FACE) experiment. By using the $\delta^{13}\text{C}$ signature in loblolly pine (*Pinus taeda*), birch (*Betula papyrifera*) and aspen (*Populus tremuloides*) from two FACE sites to monitor wood decomposition, measure the amounts of wood C incorporated into soil organic matter pools, and determine factors regulating decay processes mediated by fungi and termites within nine major forest – bioclimatic zones within the continental U.S. Our objectives are: (a) determine the influence of wood biochemistry, microbial process, soil properties, and climatic factors on log decomposition and incorporation of wood-C into mineral soil C pools; (b) determine the incidence of termite foraging, interaction between termite and fungal community activity and effects on the rate of wood decomposition and incorporation of wood C into mineral soil C pools; and (c) develop a model to simulate log decomposition and wood C movement into the mineral soil.

The work is being conducted principally on the continental-scale (FWDE), where ambient and elevated CO₂ FACE logs were placed on nine experimental forests. After six years of decay, the loss in wood density was 10-91% in aspen, 24-85% in birch, and 20-75% in pine; pine suspended above the soil to emulate standing-dead trees had the least decay 2-45%. Assays from upper 10 cm of the mineral soil affirm that the $\delta^{13}\text{C}$ signature of the FACE wood can be traced into the mineral soil. Wood-C was evident directly beneath the logs and adjacent within 50 cm. The proportion of wood C within the soil C pool varied from 3 to 9%. White rot fungi were the dominant group responsible for the wood decay.

However, the fungal community, based on DNA sequencing, exhibits distinct assemblages that appear to be related to abiotic factors. A mechanistic model, Coarse Wood Decomposition, has been developed to simulate wood decomposition, reflecting the interactions of microbial communities and arthropods, and mediated by soils, climate and vegetation attributes. The model has been parameterized for subtropical to boreal zones in North America; it is currently undergoing final testing with the FWDE data.

Poster #1-68**In the Eye of the Storm: Warmer Temperatures Affect Tropical Forest Recovery Following Hurricane Disturbance**

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Project: University Award

Hurricanes affect nearly every continent in the world and are among the most intense weather disturbances in forest ecosystems. In 2017, the coastal United States (US) and Puerto Rico were devastated by a series of major hurricanes that caused more than \$200 billion in damages, the effects of which will have long-lasting implications for the economics and natural resources of US forests. At the same time, models project that temperatures in the tropics and subtropics will increase by 3-5°C within the next 20 years. The combined effects of hurricane disturbance and warmer temperatures could fundamentally alter the trajectory and duration of forest recovery following disturbance, resulting in altered ecosystem states that are difficult to predict from historical data alone. Yet, despite both the immediate and significant effect of hurricanes on forest carbon (C) and nutrient stocks, as well as the potential to affect the long-term trajectory of forest C cycle recovery, hurricanes are not currently represented in Earth System Models (ESMs), and no studies have captured the potential interactions of hurricanes within the context of a changing climate. Here, we capitalize on a once in a century opportunity to investigate responses of key C cycling processes to experimental warming in the wake of two major Hurricanes within the Luquillo Experimental Forest in Puerto Rico. We conducted 12 months of field-level understory warming using infrared heaters arranged in six 4-m diameter plots (three +4°C heated and three control) as part of the Tropical Responses to Altered Climate Experiment (TRACE). We investigated effects of warming on soil respiration, root specific respiration, photosynthesis, and foliar respiration of understory shrubs as well as changes in root biomass and production. After one year of warming, Hurricanes Irma and Maria struck the island of Puerto Rico. We then followed forest recovery for 1-year following hurricane disturbance.

After 8 months, warmed plants showed increasing signs of stress, where increases in photosynthetic temperature optimum (T_{opt}) were less pronounced and optimum photosynthetic rates (A_{opt}) declined. Root specific respiration was significantly lower in warmed plots after 6 months of warming, demonstrating rapid acclimation to increased temperatures. At the same time, root biomass was significantly reduced but root production was not affected. Soil respiration rates were significantly higher in warmed plots. Overall, these results suggest that tropical understory plants will take up less carbon dioxide (CO₂) in a warmer world, but may also respire less CO₂ via roots, likely due to reduced belowground C allocation. While soil respiration rates increased significantly in warmed plots, root biomass was lower, suggesting increases were microbially-driven. Results could indicate a shift towards a net negative C balance in tropical forested ecosystems as global temperatures increase. Following hurricanes Irma and Maria, root production was initially reduced in warmed relative to control plots.

Interestingly, root specific respiration patterns reversed, with high root specific respiration in warmed relative to control plots. In addition, understory vegetation height was approximately 20 cm shorter in warmed relative to control plots after one year of forest recovery. These initial responses of the warmed plots to hurricane disturbance could be a consequence of reduced C cycling in warmed plots prior to disturbance.

Poster #1-33**Evaluation of High-Latitude CH₄ Emissions and their Functional Responses in the E3SM Land Model**

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Project: University Award

Climate change is a key challenge that will affect many aspects of biosphere processes. Northern high latitudes are very sensitive to warming due to ice-albedo and carbon-concentration feedbacks. In addition to permafrost soil CO₂ emissions, soil CH₄ emissions are another important factor that contribute to high-latitude warming, and these emissions are projected to increase due to soil inundation from permafrost thaw. Here we quantify Northern High latitude CH₄ production and oxidation rates in the E3SM land model (ELM). At regional scale, we conducted two sets of simulations that differ in their estimates of inundated area (prognosed and prescribed based on satellite observations). Model parameter optimization has been applied for the prognostic inundated area simulation to improve the regional scale representation of inundation. We also analyze spatial distribution and temporal evolution of soil CH₄ emissions and relate them to local environmental factors. At in situ scale, we also implemented and tested 2-D modeling capability in ELMv1 for soil thermal-hydrology-CH₄ coupling.

Terrestrial Ecosystem Science

Next Generation Ecosystem Experiments (NGEE): Arctic

Poster #1-6**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 Utqiagvik (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 CO₂ and CH₄ 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. In Phase 3 (2020 to 2022), we propose to continue our research at sites on the North Slope and in western Alaska, while also adding a cross-cutting component on disturbance. We will use field campaigns, modeling, and data synthesis 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 in Phase 3 strengthens the connection between process studies in Arctic ecosystems and high-resolution landscape modeling and scaling strategies developed in Phases 1 and 2. Safety, national and international collaboration, and a commitment to project management continue to be key underpinnings of our model-inspired research in the Arctic.

Poster #1-7**Observation-Informed Watershed-Scale Simulation of Terrestrial Processes Using ATS at the NGEE Teller Site**

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Continued warming of the Arctic system is currently driving rapid and transformative change in high-latitude landscapes. These ice-rich ecosystems are particularly sensitive to perturbations, and many of the processes that dictate system behavior are inextricably linked. For example, hydrological factors exert a dominant influence on biogeochemical processes and play a large role in determining the rates of CO₂ and CH₄ fluxes. To better understand the complex process interactions occurring as these systems change, we are simulating hydrology and permafrost dynamics in the Teller watershed with the Advanced Terrestrial Simulator (ATS). Teller watershed contains areas with near-surface, deep, and no permafrost, and can be considered to be representative of discontinuous permafrost systems. Observations suggest the watershed has an active and well-connected subsurface hydrologic system. This work utilizes many streams of observational data in a single integrated framework, providing the opportunity to refine our understanding of system behavior under current or past climatological conditions. The simulations will also serve as a numerical laboratory, allowing observations of process interactions and feedbacks in response to specific perturbations.

Poster #1-8**Vegetation-Permafrost-Hydrology-Climate Relationships Along Three Hillslopes in the Low Arctic: Synthesis of Ngee Arctic Observational Studies**

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NGEE Arctic aims to improve climate model predictions through advanced understanding of coupled processes in Arctic terrestrial ecosystems. We are synthesizing observations along three hillslopes in the low Arctic on the Seward Peninsula to expand our understanding and model representation of landscape structure and organization. Discontinuous permafrost, high annual precipitation, and well-drained watersheds characterize the three sites –Teller, Kougarok and Council – with strong topographical gradients in comparison to the high Arctic landscape of the Barrow Peninsula. Here we summarize the linkages we are in the process of identifying among vegetation, permafrost, hydrology and climate. For example, tall and dense alder and riparian shrub communities with thin organic horizons are linked to deeper winter snow depth and the presence of taliks. In contrast, shorter-stature sedge dominated communities with thicker organic horizons are associated with shallow permafrost table and low winter snowpack. Sedge dominated communities are further differentiated by soil substrate chemistry. Tussock tundra sedge dominated communities that occur on acidic soils have thinner active layers than non- acidic non-tussock sedge dominated communities. We anticipate the trends we identify will not only be useful for predictions of future ecosystem changes in the low Arctic, but will also be applicable to paleoecological reconstructions.

Poster #1-9**Characterization of Snow Distribution at Teller and Kougarok Sites of Seward Peninsula**

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Snow cover plays an important role in the climate, hydrology and ecological systems of the Arctic due to its influence on the water balance, thermal regimes, vegetation and carbon flux. Thus, snow depth and coverage have been key components in all the earth system models but are often poorly represented for arctic regions, where fine scale snow distribution data is sparse. Through the DOE Office of Science Next Generation Ecosystem Experiment, NGEE-Arctic, high resolution snow distribution data is being developed and applied in catchment scale models to improve representation of snow and its interactions with other model components in the earth system models. To improve these models, it is important to identify key factors that control snow distribution and quantify the impacts of those factors on snow distribution. Intensive snow surveys were conducted at two sites in Seward Peninsula: Teller site (in 2016, 2017, and 2018) and Kougarok site (in 2018). We built linear mixed models to explore the relationship between snow water equivalent (SWE) and different underlying controlling components including topographic factors (elevation, slope, curvature, aspect) at different spatial scales, vegetation factors (NDVI and land cover types). The results show that those factors explained 42% of the variation in snow distribution at Teller and 67% at Kougarok. For both sites, vegetation had the largest impact on the snow distribution, with more snow accumulating in the areas where the NDVI was higher and there were shrubs. In addition, snow distribution at Teller site was also largely impacted by elevation, while the snow distribution at Kougarok was also largely impacted by aspect and slope. There was strong spatial autocorrelation in the residual SWE for both sites, the snow distribution was autocorrelated at two distinct scales at Teller, 16.7m and 159.2m, while it was autocorrelated at a single scale, 44.1 m at Kougarok, reflecting the impacts of the processes and factors not explicitly considered in the linear mixed model, i.e. the local wind impact (wind drift) caused by interaction between global wind and topography and vegetation. Finally, we used our models and the spatial autocorrelation to interpolate SWE for the whole study area based on Universal Kriging method. We expect that the characterized SWE spatial distribution patterns, the statistical relationships developed between SWE and its impacting factors can be used for the development and validation of snow distribution models and to improve understanding of hydrology, vegetation and nutrient dynamics at catchment scales.

Poster #1-10**Conceptual Model of Surface Water Hydrology in Polygonal Terrain Using Stable Isotopes**

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Stable isotopes were used to characterize the timing and duration of hydrological transitions in polygonal ground at the Barrow Environmental Observatory (BEO, Utqiagvik, Alaska; 71.2956°N, 156.7664°W). Daily surface water samples were collected from 11 locations across the BEO and across arctic tundra morphologies (low centered polygon troughs (LCPTs), high centered polygon troughs (HCPTs), lakes, and drainages) during spring and summer of 2013. Previous work on the microclimatic seasons on the tundra have defined six characteristic periods based on the energy and water balances at the surface: winter, pre-melt, melt, post-melt, summer, and freeze-up. In this work, surface water stable isotopes are coupled with local climatological data (temperature, precipitation, incident/outgoing radiation, and observation) to develop a conceptual model of the dominant sources of surface water from the pre-melt period until freeze-up. At a site selected for more intensive study (HCPT), the pre-melt period surface water was dominated by snowmelt severely fractionated by winter sublimation. During the melt-period, fresh precipitation (as rain) forced runoff of the snowmelt and washed-out the remaining winter isotopic signature. The post-melt period, owing to increased incident solar radiation and reduced surface albedo, saw considerable evaporation, which correlated well with local weather observations and was noticeably punctuated by short precipitation events (exemplifying the low volume of surface water and its susceptibility to rapid change). The end of the post-melt period was characterized by a slowing of evaporation that became negligible with the beginning of the summer period. The magnitude of sublimation and evaporation processes were reconstructed using isotopic fractionation first-principals. Surface water from other morphologies (LCPTs and lakes) exhibited far less impact of sublimated snowmelt, and instead were predominately impacted by freeze-out fractionation of water that had been retained on the landscape from the previous year. One sampling location showed very little impact of either snowmelt or old-water, which suggested it was hydrologically disconnected from the low centered polygons nearby. Meanwhile, the isotopic composition of drainages were indicative of the features that supply the drainages. The spatial-temporal trends in surface water hydrology are shown to have geochemical consequences: barium, boron, potassium, and sulfate track with snowmelt, whereas calcium, magnesium, and sodium correlate with soil thaw; redox-sensitive elements are synchronized with hydrological transitions. This work improves the representation of polygonal surface water hydrology for incorporation into Earth System Models, particularly with respect to the water balance associated with the timing and duration of thawed season hydrological transitions.

Poster #1-11**Quantifying Ecosystem Functional Zones and Associated Relationships between Permafrost, Soil, Land Surface and Vegetation Properties in Arctic Systems using Geophysical Datasets**

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Understanding interactions between permafrost, soil, land surface and vegetation processes is critical for predicting the storage and flux of carbon, particularly in Arctic environments. However, quantifying above-below ground interactions is challenging due to process complexity, lack of sensing systems jointly monitoring key processes in different compartments, and the spatial variability of above-below ground interactions as a function of position within the ecosystem and season. Below we describe key advances developed during NGEE-Arctic Phase 2 to address these challenges. Advanced quantification and understanding of surface-subsurface interactions has been enabled by the development of several innovative acquisition and numerical techniques including (1) an autonomous above-below ground sensing system using pole-mounted cameras and geophysical datasets to monitor the spatiotemporal relationship between plant vigor, soil thaw depth and soil moisture, (2) a low-cost dense sensor network for Distributed Temperature Profiling (DTP) that provides unprecedented vertical and horizontal distribution of soil temperature and is adapted for integration with remote sensing data (incl., UAV), and (3) a novel inverse modeling technique that takes advantage of streaming hydro-thermal-geophysical datasets to estimate conventionally difficult to quantify properties, such as soil organic carbon. With the above novel approaches we have highlighted significant relationships between above- and belowground characteristics including: (1) the control of polygon geomorphology on soil hydro-physicochemical properties, the snow thickness, and the plant vigor at the Utqiagvik site, (2) the effects of topography and vegetation on snow depth, and with subsurface characteristics on the distribution of near-surface permafrost and taliks in warm permafrost environments, and (3) the significant influence of soil hydrological and thermal behavior on the biogeochemical CO₂ and CH₄ fluxes. Using the newly developed relationships between permafrost, soil, land surface and vegetation processes, as well as the identification of distinct ecosystem functional zones, we documented how localized ground based ‘point’ measurements can tractably be scaled to landscape scales. For example, we integrated net ecosystem exchange (NEE) measurements acquired using sparse ground-based chambers with collocated time-series of normalized difference vegetation index (NDVI) and with spatially extensive airborne LiDAR and NDVI datasets to estimate C fluxes as a function of polygon-based zones. Overall, advances and integration of new sensors and inversion approaches and ecosystem zonation construct has allowed us to quantify how complex Arctic systems behave at local scales as well as their aggregated responses at landscape scales. The obtained information is expected to be useful for improving predictions of Arctic ecosystem feedbacks to climate.

Poster #1-12**Characterizing Sources and Sinks of CO₂ and CH₄ Across Polygonal Tundra: A Multi- Scale Approach**Sigrid Dengel^{1*}, Jovan Tadic¹, Ori Chafe^{1,2}, and Margaret Torn¹¹ Lawrence Berkeley National Laboratory, Berkeley, CA;² University of Oregon, Eugene, ORContact: SDengel@lbl.gov

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Identifying sources and sinks of carbon dioxide (CO₂) and methane (CH₄) fluxes in heterogeneous Arctic ecosystems, such as polygonal tundra, represents challenges not experienced in lower latitudes. Polygons, ice-wedge features that result from cycles of freezing and thawing of the active layer can extend several tens of meters across. Polygons at the NGEE Arctic Utqiagvik (formerly Barrow) Alaska site can be categorized as high-centered, low-centered, and flat-centered polygons, each representing different micro topography and hence surface, soil, and hydrological properties. We are measuring net CO₂ and CH₄ fluxes at landscape level with an eddy covariance (EC) tower. While data are sampled many times per second, they are typically averaged to half hourly values. However, these ecosystem scale fluxes can be temporally “dissected” to locate or identify localized sources and sinks on the order of less than 5 m. We are attempting to localize these fluxes by combining a variety of measurements methods and techniques to better understand the carbon and energy budgets of this complex environment. To do so we employ refined geostatistical and geospatial analysis by integrating a high resolution elevation model to identify and extract individual polygons by type and extend (60 polygons were surveyed (Wainwright et al. 2015) and are used as ground truthing), combined with stationarity tested 5-min averaged EC data with accompanying footprint analyses (fetch distance of up to 250 m – wind direction and atmospheric stability dependent), bivariate polar plots and cluster analysis in order to depict seasonal and inter-annual photosynthetic properties of individual polygons and polygon types in regards to environmental changes (wet vs dry, cold vs. warm growing seasons). Once these high-resolution, multi-layered datasets have been assembled we are then amalgamating them by applying sophisticated machine learning techniques in order to advance our understanding of these ecosystems, which can be implemented into earth system models and improve the fidelity of model predictions.

Wainwright et al. (2015). Identifying multiscale zonation and assessing the relative importance of polygon geomorphology on carbon fluxes in an Arctic tundra ecosystem. *Journal of Geophysical Research: Biogeosciences*, 120(4), 788-808.

Poster #1-13**Topographic and Climatic Controls on Peri-Glacial Hillslope Sediment Transport: A Regional Study of Solifluction**Mulu Fratkin^{1*} and Joel Rowland¹¹ EES-14, Los Alamos National Laboratory, Los Alamos, NMContact: mfratkin@lanl.gov

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Solifluction lobes, the downslope transport of soil in discrete lobes, are ubiquitous features of periglacial and alpine landscapes throughout the world. In Alaska and across the Arctic, the creep of soil driven by freezing and thawing cycles creates patterned roughness elements that dominant entire hill-slopes. The impact of solifluction on the microtopography of hillslopes can result in feedbacks between vegetation, snow-cover, and hillslope erosion. Solifluction lobes also act to redistribute carbon on hillslopes by continually burying vegetation, altering flow pathways, and transporting organic rich mats of sediment towards colluvial hollows and valley bottoms. However, the occurrence of solifluction is highly sporadic due to the strong dependencies on local climate, geology, and hydrology conditions. A large body of literature investigates the structure and rate of solifluction lobes at the scale of a single lobe or hillslope. Few studies investigate solifluction at a regional scale and those that do typically implement probability models to capture where solifluction might occur with no information related to the morphology of lobes. In this study we incorporate a suite of new datasets for the country of Norway as the availability of topographic data at a sufficient resolution to resolve solifluction lobes is highly limited in the arctic, including Alaska. We incorporate three primary datasets in this analysis: 1) high resolution (1m) LiDAR derived digital terrain models, 2) Gridded (1km²) temperature data on daily and hourly intervals and 3) displacement estimates derived from InSAR processing techniques. Given the wide coverage of all three datasets, we identify more than 50 hill-slopes exhibiting significant solifluction allowing us to delineate over 300 individual solifluction lobes using automated and manual methods. The North-South orientation of Norway results in hill-slopes covering a wide range of latitudes including permafrost and non-permafrost landscapes. With this dataset we will be able to identify the controls on the occurrence and morphology of solifluction lobes at a range of spatial scales and as a function of hill-slope steepness, aspect, and elevation as well as annual fluctuations in surface air temperature. Based on this study, we will be able to map likely distributions and characteristics of hillslope microtopography in regions, such as Alaska, lacking extensive high-resolution topographic datasets.

Poster #1-14**Estimation of Soil Properties by Coupled Inversion of ERT and Hydrothermal Measurements**

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Studies indicate greenhouse gas emissions following permafrost thaw will amplify current rates of atmospheric warming, a process referred to as the permafrost carbon feedback (PCF). However, large uncertainties exist regarding the timing and magnitude of the PCF, in part due to uncertainties associated with subsurface parameterization. Development of robust parameter estimation methods is becoming urgent under accelerated warming of the Arctic. Improved parameterization of the subsurface properties in land system models would lead to improved predictions and reduction of modeling uncertainty. We developed a parameter estimation (PE) framework by utilizing the PEST (Model Independent Parameter Estimation and Uncertainty Analysis) toolbox and coupled hydro-thermal-geophysical modeling. The main goal of this study is to demonstrate the proof-of-concept by testing the parameter estimation framework against synthetic data. We use known subsurface parameters and coupled models to set up a synthetic state, then perturb the values of those parameters using our PE framework to recover the synthetic state. We consider a set of perturbed subsurface properties as a sample that consists of multiple sets of perturbed parameter values. The convergence is robust if most of the perturbed values from the sample are able to converge to their synthetic state. We evaluate the type and amount of data needed to allow the best convergence. In addition, we provide recommendations on the value and design of subsurface observations based on the results of our synthetic studies.

Poster #1-15**Evaluating Soil Thermal Hydrology Models Against Field Observations in Arctic Polygonal Tundra**

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Numerical simulations are essential tools for understanding the complex hydrological response of the Arctic regions to a warming climate. However, strong coupling among thermal and hydrologic processes on the surface and in the subsurface and the significant role that subtle variations in surface topography have in regulating flow direction and storage within a polygon lead to significant uncertainties. Careful model evaluation against field observation is thus important to build confidence. Here, we evaluate the Advanced Terrestrial Simulator (ATS) (Coon et al. 2016; Painter et al. 2016) against field observations in polygonal tundra at the Barrow Environmental Observatory. ATS represents important physical process such as lateral surface and subsurface flows, advective heat transport, cryosuction, and coupled surface energy balance. We conducted two- and three-dimensional simulations on generic surface microtopography considering radial symmetry of ice-wedge polygons. We drove the simulations with meteorological data and observed water table elevations in polygon troughs, and compared simulated water table elevations in the polygon centers to observed values. The simulations were found to be sensitive to parameters in the bare-soil evaporation model, the soil horizontal hydrologic conductivity, and trough-to-rim elevation difference. With modest amount of calibration of the soil properties and evaporation model parameters, the simulations were found to be consistent with observed water tables, active layer thickness, and observed soil temperatures at several depths in trough, rim, and center. This study demonstrates the improved representation of important process such as soil moisture, evaporation and thawing, and identifies a set of parameters for watershed-scale models.

Painter SL, ET Coon, A Atchley, M Berndt, R Garimella, JD Moulton, D Svyatskiy, and CJ Wilson. (2016). Integrated surface/subsurface permafrost thermal hydrology: Model formulation and proof-of-concept simulations. *Water Resources Research* 52: 6062-6077.

Coon ET, JD Moulton, and SL Painter. (2016). Managing complexity in simulations of land surface and near-surface processes. *Environmental Modelling & Software* 78: 134-149.

Poster #1-16**Interactions Between Climate Warming and Fire Will Drive Expansion of High-Latitude Deciduous Vegetation**

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High-latitude regions have experienced the most rapid warming in recent decades and this trend is projected to continue over the 21st century. Fire is also projected to increase with warming. We show here, consistent with changes during the Holocene, that projected changes in 21st century climate and fire will also alter the modeled composition of Alaskan vegetation. We hypothesize that tradeoffs in competition for nutrients after fire in early succession versus for light later in succession under warmer climate will cause shifts in plant functional types (PFTs). Consistent with observations, evergreens were modeled to be the current dominant PFTs in Alaska. However, under future climate and fire the relative dominance of deciduous PFTs will double from current levels, accounting for 58% of Alaska ecosystem net primary productivity (NPP) by 2100, with commensurate declines in contributions from evergreens and herbaceous plants. Post-fire deciduous PFTs growth under future climate was sustained from enhanced microbial nitrogen mineralization caused by warmer soils and deeper active layers, resulting in taller plants that competed more effectively for light. Expansion of deciduous PFTs will affect the carbon cycle, surface energy fluxes, and ecosystem function, thereby affecting multiple feedbacks with the climate system.

Poster #1-17**Modeling Soil Temperature Change in Seward Peninsula, Alaska**

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We apply an ecotype-based modeling approach to model high-resolution permafrost dynamics in the Seward Peninsula - an NGEE-Arctic study region with highly vulnerable warm discontinuous permafrost in the Western Alaska. We use a transient soil heat transfer model developed at the Geophysical Institute Permafrost Laboratory (GIPL-2) to compute temperature dynamics in the ground material. The model solves one dimensional nonlinear heat equation with phase change and assumes the unfrozen liquid water content in soil pores. The spatially distributed model is forced with combination of historical climate and different future scenarios for 1900-2100 with 2x2 km resolution prepared by Scenarios Network for Alaska and Arctic Planning (www.snap.uaf.edu/). Vegetation, snow and soil properties are calibrated according to the ecotype cover and are up-scaled using the Alaska Existing Vegetation Type map for Western Alaska (Fleming, 2015) with 30x30 m resolution provided by Geographic Information Network of Alaska (<http://akevt.gi.alaska.edu>). A data assimilation technique is applied to recover thermal properties for each ecotype using available observations of air, surface and sub-surface temperatures and snow cover collected by various agencies and research groups (e.g. NGEE, USGS, UAF, USDA). The applied calibration approach considers a natural variability between stations in the same ecotype and finds an optimal set of model parameters for snow and soil within the study area. This approach allows reduction in microscale heterogeneity and aggregated soil temperature data from shallow boreholes which is highly dependent on local conditions. Because of this study we present a series of preliminary high-resolution maps for the Seward Peninsula showing changes in the active layer depth and ground temperatures for the current climate and future climate change scenarios. The modeling results are to be improved within the next NGEE phase.

Fleming MD. (2015). Developing an existing vegetation layer for the Western Alaska LCC region. Technical report, <http://akevt.gi.alaska.edu>.

Poster #1-18**Hillslope Biogeochemistry Controls on Anaerobic Soil Organic Matter Decomposition in a Tundra Watershed**

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We investigated rates and controls on greenhouse gas production in two contrasting water-saturated tundra soils within the Teller Road mile 27 watershed near Nome, Alaska. Three years of field sampling have shown that soil from a fen-like area at the base of the hillslope had higher pH and higher porewater ion concentrations than soil collected from a bog-like peat plateau at the top of the hillslope. The influence of these contrasting geochemical environments on CO₂ and CH₄ production was tested by incubating soil microcosms anaerobically at -2°C and 8°C for 55 days. NH₄Cl was added to half of the microcosms to test the effects of N limitation on microbial greenhouse gas production. We found that total CO₂ and CH₄ production were higher in the soils from the bottom of the hillslope. Water-extractable organic C (WEOC) was also higher in these soils, and fermentation of this C pool resulted in an increasing supply of low-molecular weight organic acids (e.g., acetate and propionate) throughout the incubations. Higher availability of labile DOC, in addition to higher pH, likely contributed to the more rapid greenhouse gas production at the bottom of the hillslope. Our results also indicate that inorganic N concentrations were lower and soil C decomposition was more N-limited in the peat plateau soils than the soils from the bottom of the hillslope, which exhibited net N mineralization while the peat plateau soils had net N immobilization. Nitrogen addition increased CO₂ production in the peat plateau soils but not the lowland soils, consistent with greater N limitation. Our results suggest that the movement of water, ions, and nutrients down the tundra hillslope can increase the rate of anaerobic soil organic matter decomposition by (1) increasing the pH of soil porewater; (2) providing bioavailable DOC and fermentation products such as acetate; and (3) relieving microbial N limitation through nutrient runoff.

Poster #1-19**Topographical Controls on Hillslope-Scale Hydrology Drive Shrub Distributions on the Seward Peninsula, Alaska**

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Shrubs are expanding across the Arctic tundra in response to warming, and topography and landscape hydrology are key controls of the spatial distribution of vegetation changes. Observations have shown that shrub expansion is located mainly on hillslopes, although the processes through which topography controls shrub expansion remain unclear. To examine hydrological controls on shrub distributions, we applied a coupled transect version of a mechanistic ecosystem model (*ecosys*) at the NGEE-Arctic Kougarak Alaska hillslope site, which is underlain by impermeable permafrost. Modeled distributions of the dominant plant functional types and aboveground biomass across the hillslope agreed very well ($R^2 > 0.85$) with measurements in 2016. Modeled differences in soil water content across the slope during the growing season were driven by variations in total soil water holding capacity and lateral water flow. In the well-drained upper slope position of the hillslope, plant N-uptake was modeled to be low from microbial water stress (and thus lower N mineralization), resulting in smaller modeled plant biomass. Intermediate soil moisture in the middle slope position enhanced mineralization and plant N uptake, and thus plant biomass. The gentle slope and deeper soil in the lower slope position resulted in saturated soil conditions, reduced root and microbial O_2 uptake, and thus lower biomass. A simulation ignoring topography (i.e., a flat landscape with the same soil properties, plant and microbial traits, and climate forcing) over- or under-estimated (depending on hillslope position) vegetation productivity. Overall, the mean shrub NPP across the transect was underestimated by 34% in the flat landscape compared to the realistic interconnected grids across the slope gradient. Our results indicate that land models that do not account for hillslope- scale surface and sub-surface flows of water, nutrients, and energy may not accurately predict plant distribution changes in Arctic ecosystems.

Poster #1-20**The Response of Photosynthesis and Respiration to Experimental Warming in the High Arctic**

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The temperature in the Arctic has increased by more than twice the global mean temperature and will continue to rise rapidly over the next century. The high sensitivity of the Arctic to climate change coupled to the increasingly important, yet uncertain role Arctic ecosystems are playing in the global carbon cycle, emphasizes the need to advance understanding and model representation of ecosystem processes and fluxes in the Arctic. Understanding plant photosynthesis and respiration is central to closing this knowledge gap. The Farquhar, von Caemmerer and Berry (FvCB) model of photosynthesis is at the heart of many Terrestrial Biosphere Models (TBMs) yet we lack key information that can enable robust projections of the response and acclimation of key model parameters, such as maximum carboxylation rate, to projected warming in the high Arctic. We also lack the technology necessary to manipulate growth temperature *in situ* and enable the collection of data required to close this knowledge gap. To address this, we developed a novel method for warming the tundra that is focused on advancing understanding of key leaf level plant physiology for implementation in TBMs. Our zero-power warming (ZPW) chambers use passive warming and modulated venting to elevate the thaw season air temperature by ~4°C above ambient. Each year we move our ZPW chambers to new locations to capture different vegetation – focusing on stands that are large enough to support repeated measurement and sampling. We are currently half way through a four-species, four-year data collection effort. Here we present data on the response of photosynthesis and respiration to elevation of thaw season temperature from the first two species we have investigated; *Petasites frigidus* (forb) and *Arctagrostis latifolia* (grass).

Poster #1-21**Effects of Short-Term Warming on Allocation and Nutrient Acquisition in an Arctic Grass**

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Project: Ngee Arctic

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

Arctic ecosystems are warming rapidly and are expected to reach hot extremes more frequently in the coming decades. Nitrogen (N) and phosphorus (P) availability are low in the arctic and these nutrients are known to limit the productivity of tundra plants more directly than temperature. To better understand the relationship between temperature and nutrient cycling within arctic plants and soils, we investigated the impact of short-term warming on soil nutrient availability, plant N uptake, and plant N allocation. A warming treatment was implemented in Utqiagvik, Alaska on the Northern coastal plain using Zero Power Warming (ZPW) chambers that elevated air temperatures by 4°C (n=5) during the 2018 growing season. Ion-exchange resins were deployed from June-September to assess availability of inorganic N and P in surface soils. An injection of tracer ¹⁵N-NH₄ was performed at 3 cm depth in July and left for one week (+200 mg N/ m²). At this point in the growing season, the ZPW treatment was increasing soil temperature at 5 cm depth by ~1°C. At the end of one week, harvests of 9 × 9 cm squares of tundra were performed, targeting labeled and unlabeled patches of the grass *Arctagrostis latifolia*. Back in the laboratory, *A. latifolia* biomass was sorted into blades, sheaths, inflorescences, attached litter, rhizomes, and fine roots. Rates of ¹⁵N-NH₄ uptake will be determined by comparing the 15N content of tissues from labeled and unlabeled tissues. Initial results suggest P availability in surface soils has increased with warming. Aboveground biomass of *A. latifolia* was not impacted by warming treatment, nor were aboveground traits associated with productivity (height, specific leaf area, leaf area index, leaf %N, leaf N mass per unit area). Chemical analysis of aboveground tissues, however, showed warmed plants have decreased %N within inflorescences (p=0.01) which could be due to warmed plants developing a larger and more mature pool of inflorescences. Belowground fine-root data is still forthcoming, but rhizome data suggest warming is associated with thinner rhizomes, potentially indicating a warming-induced increase in lateral growth. Under warmed conditions, *A. latifolia* also had significantly higher atom percent enrichment in live, aboveground tissues (p=0.02) with the greatest differences observed in sheaths and blades. These preliminary findings suggest that a single growing season of elevated temperature can increase soil nutrient availability, alter plant N allocation, and impact the development of key plant tissues.

Poster #1-22**How Variations in Vegetation Cover, Micro-topography, and Snow Depth Impact Soil Temperature and Respiration in an Arctic Watershed**

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Arctic ecosystems are characterized by fine-scale heterogeneity of surface and subsurface structure, with differences in hydrological conditions, soil physical properties, and vegetation cover strongly influencing the distribution of soil carbon content and fluxes across a watershed. This spatial variation poses a unique challenge to upscale soil carbon content and flux measurements from the sub-watershed scale to the regional scales that are used in full-scale climate models. This study focuses on understanding links between surface and subsurface controls on thermal and biogeochemical regimes, and how such links can be used to improve the representation of carbon and nitrogen cycling during the fall and early winter (late shoulder season) in ecosystem models. At a discontinuous permafrost site in a Seward Peninsula watershed near Council, AK, low-altitude Unmanned Aerial System (UAS) images and ground-based measurements were used to investigate links between surface and subsurface properties. UAS-inferred multi-spectral images and a Digital Surface Model (DSM) were used to perform a vegetation classification and hydrological stream flow analysis, and these products were compared with measurements of soil temperature, soil electrical conductivity, and respiration sampled using dark gas flux chambers at multiple points and across multiple years. We found that complex micro-topographical features lead to large inter-site variations in surface wetness regimes that influence vegetation distribution, creating ecotypes that can be distinguished using remotely sensed products and which are characterized by distinct subsurface thermal regimes and methane emissions. Snow packs across the Seward Peninsula were unusually deep during the winter of 2017-2018, contributing to appreciably warmer near-surface soil temperatures the following spring. We found that variations in snow pack depth had the largest effect on interannual variations in growing-season carbon fluxes at the end of the season. In addition, 1-D simulations of water, heat and CO₂ fluxes under the observed atmospheric forcing were performed using *ecosys*, a mechanistic terrestrial ecosystem model. These simulations were used to perform analyses of the effect of soil composition, vegetation cover, and precipitation on subsurface thermal regimes and biogeochemical processes. These simulations show that high snow packs lead to warmer soil temperatures and enhanced CO₂ fluxes during the following late shoulder season. Field data and simulations show that this effect is particularly important in patches of tall shrubs and in micro-topographic lows.

Poster #1-23**Refining ELM Simulations of Arctic Field Sites Using Vegetation Community and Biomass Measurements**

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Land surface models, including the E3SM Land Model (ELM), conceptualize plant communities using mixtures of plant functional types (PFTs) with fixed parameter values. PFT definitions and parameters defined in the context of global simulations often do not correspond well with plant communities at the scale of individual sites. This is an especially important issue in Arctic ecosystems, where plant communities vary over small spatial scales and are often dominated by grass, shrub, moss, and lichen vegetation types that are not well represented in global models. We used a combination of plant community surveys and biomass measurements to define and parameterize plant communities specific to the Kougarak field site, located on the Seward Peninsula and part of the Ngee-Arctic field program. The Kougarak site encompasses a range of ecotypes, including alder shrubland, tussock tundra, and rocky areas dominated by dwarf shrubs and lichens. We defined new arctic-specific PFTs within ELM, including dwarf evergreen shrubs, arctic mosses, and arctic grasses, and modified their allometric and stoichiometric parameters based on site measurements of biomass, productivity, and tissue stoichiometry.

Compared to model simulations using baseline ELM parameters, site-specific PFTs and parameterizations yielded more accurate simulations of canopy height, total biomass, aboveground-belowground partitioning of biomass, and annual net primary production. Differences in plant communities and vegetation traits across the Kougarak site led to variations in both total vegetation biomass and soil carbon stocks that could not be reproduced using baseline ELM PFTs. Simulations with updated PFTs also produced significantly different ecosystem-level responses of biomass and soil carbon to projected warming scenarios at the Kougarak site. These results highlight the value of site-specific vegetation measurements for developing accurate simulations of current and future carbon and nutrient cycling in arctic ecosystems.

Poster #1-24**A Mechanistic Explanation of the Hysteretic Temperature and Moisture Dependence of Soil Carbon Decomposition Dynamics**Jinyun Tang*¹ and William J. Riley¹¹ Lawrence Berkeley National Laboratory, Berkeley, CAContact: jinyuntang@lbl.gov

BER Program: TES, ESM

Project: NGEA Arctic and E3SM

Project Website: <https://ngee-arctic.ornl.gov/>; <https://climatemodeling.science.energy.gov/projects/energy-exascale-earth-system-model>

Understanding and modeling how temperature and moisture regulate soil carbon decomposition is of paramount importance for the prediction of biogeochemistry-climate feedbacks. Existing theories have often represented the temperature and moisture effects using multiplicative factors, implicitly assuming that biogeochemical reaction, temperature, and moisture controls are linear in the logarithm space, although, in reality, the three are always entangled. Here we present a first-principle based formulation of how temperature and moisture influence biogeochemical reactions through their modulation of substrate transport, uptake, organic-mineral interaction, and microbial dynamics. We evaluated our model predictions with incubation and field data synthesized across a wide range of soils. We demonstrate that temperature and moisture interact non-multiplicatively in modulating biogeochemical reactions and consequently soil carbon decomposition dynamics. We show that many of the temperature and moisture response curves used in current models are consistent with specific environmental conditions over the observation period, but not for the much wider range of current and expected environmental variability. Under transient and variable environmental conditions, the temperature and moisture responses are hysteretic and much more variable and are difficult to represent accurately as deterministic and multiplicative functions. By resolving the more abundant spatiotemporal dynamics, our theory therefore has a great potential to significantly improve prediction of soil carbon dynamics and their interactions with climate.

Poster #1-25**Seasonal Dynamics of Arctic Tundra Microbes**

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Arctic soils are one of the world's largest terrestrial carbon storages thus an important focal point for climate change research. With increasing global temperatures, arctic soil carbon stores may become available for rapid microbial mineralization and result in increased greenhouse gas (GHG) emissions. Different landscape features in soil surface and subsurface such as slope, redox gradients, ice wedge formation, depth of permafrost can result in diverse microbial habitats that might respond differently to warming and perturbations. Seasonal changes in soil microbiomes and its impact on GHG production potential is not well understood. In this project, we applied metagenomics and microarrays (GeoChip) to determine the phylogenetic and functional differences in the active layer soil microbiomes from two NGEE-Arctic field sites: polygonal arctic tundra at the Barrow Environmental Observatory (BEO) and a watershed (Teller Rd) nearby Nome in Seward Peninsula. In BEO, Arctic tundra microbiomes are structured along topographical features. This structuring had a direct impact on distribution of key genes for GHG emissions where GHG production potential was localized and showed large variations between different polygons. Microbial genomes showed improved resilience to changes in carbon availability, fluctuating temperatures and nutrient-deficient conditions in tundra soils. Even though microbiomes showed seasonal variations; over a thaw season landscape topography remained as a main distinguishing factor for distribution of microbial functions. Landscape topography in hill slopes of Teller Rd watershed, was also a strong determinant for soil geochemistry, vegetation distribution, soil microbiomes and GHG fluxes. In this field site besides topography, nutrient availability and pH were strongly correlated with soil microbiomes and GHG fluxes. We are currently developing statistical models to determine relationships between microbial activity, competition for resources and topography. Integrating microbial functions with geochemistry and GHG fluxes aids us in determining the impact of landscape topography in biogeochemical cycles in Arctic soils and in the future, these efforts will contribute to resolving uncertainties surrounding ecosystem responses.

Poster #1-26**Integrated Modeling for NGEE-Arctic Phase 3: New Modules of Predictive Capability for E3SM**

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Phase 3 of the NGEE-Arctic project will have as a primary modeling goal the integration of multiple modules of new predictive Arctic tundra capability within the E3SM Land Model (ELM). This goal builds on extensive fine-scale and intermediate-scale modeling capabilities already developed by NGEE-Arctic, and provides a direct pathway for climate-scale integration of new observational and experimental knowledge gained within the question-based NGEE- Arctic research areas. Six specific areas are being targeted for new predictive modeling capabilities within ELM: 1) representation of sub-grid inundation fraction, and the influence of inundation on other thermal, hydrologic, and biogeochemical processes; 2) Improved parameterization of sub-grid hillslope processes to capture variation in atmospheric forcing as well as hillslope process connectivity; 3) interactions of snowpack with surface weather, terrain position, and vegetation structure, and the influence of varying snowpack on thermal, hydrologic, and biological processes; 4) representation of alder as a unique component of the Arctic shrub tundra community, including its roles in nutrient cycling; 5) improved predictions of pan-Arctic dynamic biogeography to represent future distributions of vegetation types and traits; and 6) improved representation of the oxic/anoxic transitions in Arctic tundra soils and the influence of these on other biogeochemical processes. Examples of foundational work in each of these areas is presented, along with forward-looking descriptions of how these new modules will be incorporated in ELM, and the expected outcomes for regional, pan-Arctic, and global climate system predictions.

Poster #1-27**Very Old and Very New Soil Organic Carbon in the Arctic is Equally Sensitive to Warming: ¹⁴C Evidence in the NGEA Arctic Project**

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The Arctic is expected to shift from a sink to a source of atmospheric CO₂ this century due to climate-induced increases in soil carbon mineralization. The magnitude of this effect remains uncertain, however, largely because temperature sensitivities of organic matter decomposition and the distribution of these temperature sensitivities across soil carbon pools are not well understood. We used a novel analytical method with natural abundance radiocarbon (¹⁴C) to evaluate temperature sensitivities across soil carbon pools. With soils from Utqiagvik (formerly Barrow), Alaska, we used an incubation experiment to evaluate soil carbon age and decomposability, disentangle the effects of temperature and substrate depletion on carbon mineralization, and compare temperature sensitivities of fast-cycling and slow-cycling carbon. Old, historically stable carbon was shown to be vulnerable to decomposition under warming. Using radiocarbon to differentiate between slow-cycling and fast-cycling carbon, temperature sensitivity was found to be invariant among pools, with a Q₁₀ of ~2 irrespective of native decomposition rate. These findings imply that mechanisms other than chemical recalcitrance mediate the effect of warming on soil carbon mineralization. This work also informs land models of arctic biogeochemistry, showing that carbon age or pool turnover time does not constrain the temperature sensitivity. Even very old yedoma or buried carbon in the Arctic may be vulnerable to rapid decomposition upon thaw or warming.

Poster #1-28**Understanding Controls on Soil Moisture Using In-Situ TDR, Airborne SAR and UAS Lidar Data at the NGEE-Arctic Teller Field Site**

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NGEE-Arctic scientists are analyzing in-situ and multi-scale remote sensing data to understand interactions between surface and subsurface landscape structure and the spatial distribution of soil moisture across the NGEE Arctic Teller road field site. The work aims to demonstrate an approach to extend local soil moisture observations to watershed and regional scales for use as model benchmark datasets. We co-analyzed simultaneous observations from NASA's Arctic Boreal Vulnerability Experiment (ABOVE) airborne synthetic aperture radar (SAR) August 2017 campaign, with NGEE-Arctic's unmanned aerial system (UAS) lidar intensity data and *in-situ* measurements of soil moisture to produce a high-resolution map of distributed soil moisture. We further examined how local geomorphology, topography, climate and vegetation properties interact with soil moisture patterns within the watershed. In situ soil moisture data was collected with a Hydrosense-II soil-water sensor and data logger which uses time domain reflectometry (TDR) and the dielectric properties of the soil to estimate volumetric moisture content. Data were collected along transects located within 100m by 100m plots following a standard ABOVE protocol. UAS lidar intensity data shows a unique signature for standing water, and provides a watershed-wide, high-resolution (0.1m) map of potential saturated areas. The spatially sparse in-situ data was combined with the spatially coherent lidar intensity data to interpret and convert Airborne SAR data into a map of spatially distributed soil moisture. This analysis provides a unique benchmark dataset with which to test predictions of spatial variation and temporal evolution of soil moisture in local and regional permafrost models.

Poster #1-29**Preliminary Assessment of E3SM Land Model (ELM) in Northern High-Latitude Regions and Its Improvements by MODEX Approach**

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In high-latitude Arctic, modeling land surface processes are of great challenge in Earth System, mostly due to highly heterogeneous surface across scales and lacking data in those remote and harsh regions. In this study, we present an offline land surface simulation using the newly developed Energy Exascale Earth System Model's (E3SM) Land Model (ELM) over northern high-latitude regions (>60°N) at half-degree spatial resolution. As a benchmark, ELM simulated vegetation and soil organic matters are evaluated. Further improvement aiming to high resolution modeling via model development and experiment data integration (MODEX) are explored in the Next Generation Ecosystem Experiment-Arctic (NGEE-Arctic) Intensive Study Sites. By using ILAMB tools and available datasets, it shows that ELM simulation of vegetation LAI and total soil organic matter (SOM) improved remarkably, compared to its precedent CLM, but still mismatch both spatially and temporarily. As demonstration, we collected model driving forcing data either from local meteorological station (Utqiagvik, AK) or high-resolution DAYMET product (Kougarok, Seward Peninsula, AK) for two NGEE-Arctic field sites. Simulations are much more comparable to data. Plant physiological parameters and vegetation distribution from field surveys are also highly valuable to high resolution modeling, as shown by incorporating field measurements into ELM. Identifying and integrating those physical and physiological properties and featuring them in model frameworks appropriately with spatial resolutions, is critical to capturing biosphere-atmosphere exchanges at various scales. Further improvement may be achieved by incorporating 3-D reactive-transport model, e.g. PFLOTRAN, as demonstrated in this study as well, because of its much better representation of nutrient transport processes.

Terrestrial Ecosystem Science

Next Generation Ecosystem Experiments (NGEE): Tropics

Poster #1-42**Next-Generation Ecosystem Experiments (NGEE)–Tropics Overview**

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Tropical forests cycle more CO₂ and water than any other biome and are critical to Earth's energy balance. Yet processes controlling tropical forest carbon cycling are not well established, and large uncertainties in observational estimates and Earth system model (ESM) projections of net carbon fluxes remain unresolved, contributing significant uncertainty to climate projections. 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 develop an 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 (i.e. ModEx) is our fundamental approach toward attaining this goal, with our grand deliverable a representative, process-rich tropical forest ecosystem model, 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 ESM grid cell.

Phase 1 research focused on developing an improved understanding and model representation of key tropical forest processes including: responses to changing temperature, precipitation, and atmospheric CO₂; disturbance and land-use change; and heterogeneity in belowground processes. NGEE-Tropics developed a transformational, process-rich model framework called the Functionally Assembled Terrestrial Ecosystem Simulator (FATES), which was integrated into DOE's Energy Exascale Earth System Model (E3SM), and further model development and measurement activities were integrated at pilot study field sites in Puerto Rico, Brazil, and Panama. A data synthesis and management framework was developed and continues to provide data products via a community portal.

Phase 2 will further develop and strengthen our use of FATES within E3SM as the central modeling framework that integrates our research. Process representation in FATES will be organized across three scales: processes at the scale of individual plants (cohorts), processes at the scale of competitive interactions among cohorts (landscape), and large-scale coupled processes (regional).

Poster #1-43**A Synthetic Community Approach to Understanding Root-Bacterial Interactions During Drought in *Clusia pratensis***

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Models increasingly predict a rise in the severity and duration of drought events, which threaten tropical forests and the role they play in global cycles. Roots serve as the interface between plant and soil, but roots also host a rich and diverse microbial community, which contain functional traits that complement root nutrient and water uptake. Efforts to untangle the interactions between roots and microbial communities and relate them to plant fitness have been hampered by the inherent complexity in natural ecosystems. Thus, we designed synthetic microbial communities to study how combinations of microbial functions may affect root traits in drought conditions and what this might mean for tropical forests in a changing world.

Our synthetic communities consist of bacterial isolates collected from Luquillo Experimental Forest in Puerto Rico. Approximately 100 bacterial isolates were screened for the highest activities in four functions considered beneficial to plant growth: phosphatase activity, phosphorus solubilization, indole-3-acetic acid (IAA) production, and drought tolerance. We created four different communities of bacterial isolates and inoculated them onto *Clusia pratensis*, a tropical tree species (n = 10 plants for each constructed community). Drought conditions were imposed on half the plants for 2 months in a randomized block design and bi-weekly measurements of gas exchange were taken along with leaf samples for physiology assays and soil samples for microbial DNA extraction and analysis. Roots were harvested at the end of 2 months for biomass, phosphatase activity, length, and diameter.

The drought treatment predictably drove the largest differences between plants regardless of the inoculated constructed community. Leaf assays of membrane damage (lipid peroxidation) and stress (proline concentration) show a strong divergence mid-way through the drought trial ($p < 0.001$), indicating strong drought stress in droughted plants. However, there was no effect of microbial community composition on leaf stress response. Biomass was significantly higher in watered plants ($p < 0.001$), but not between microbial communities. Drought plants inoculated with drought tolerant and IAA producing isolates had 36% higher root biomass relative to drought plants grown in sterilized soil (control). Similarly, drought plants inoculated with high phosphatase and P solubilizing isolates showed 55% higher root biomass when compared to the control. These results suggest that microbial communities benefit plants through influencing root growth and nutrient acquisition, which may extend drought tolerance. Next steps include measuring root traits and sequencing the soil collected throughout the trial in order to determine how our synthetic communities changed throughout the trial and whether those changes can be matched to leaf and root physiological status.

Poster #1-44**A Novel Forest Regeneration Submodel for Vegetation Demographic Models**

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Earth system models are used to project the fate of forests in response to climate and land use change. They are increasingly adopting vegetation demographic modeling approaches that explicitly represent tree growth, mortality, and recruitment, enabling advances in the projection of forest resilience and vulnerability. Despite recent progress in the representation of vegetation demographics, explicit representation of forest regeneration processes, such as flower and seed production, seed longevity, seedling dynamics, and sapling recruitment have largely been neglected in these (and earlier) models. This is despite the central importance of regeneration in mediating key ecological phenomena under global change: compositional turnover, post-disturbance trajectories of forest recovery, and geographic range shifts. Here we present a regeneration submodel that improves current representations of forest regeneration processes in a format compatible with vegetation demographic models (VDMs). The submodel explicitly and efficiently represents allocation to reproduction, seed bank dynamics, seedling dynamics, and recruitment into the adult population. It has been formulated and parameterized for seasonally dry tropical forests using data from Barro Colorado Island. The model includes four plant functional types that vary in shade and soil moisture tolerance. This model demonstrates PFT-specific size-dependent reproductive allocation, soil-moisture-dependent seedling emergence and mortality, light-dependent seedling mortality, and light-dependent recruitment rates. At BCI the submodel has reduced biases in VDM-predicted recruitment rates, simulated observed seasonality of seedling emergence and interannual trends in recruitment. Adam is currently working on model sensitivity analyses and testing the model at new sites to evaluate model performance and biogeographic generalizability.

Poster #1-45**Tropical Ecological Forecasting for ENSO Using a Global Modeling Framework**Forrest Hoffman^{1*}, Paul Levine², Min Xu¹, Nathan Collier¹, and James T. Randerson²¹ Oak Ridge National Laboratory, Oak Ridge, TN;² University of California Irvine, Irvine, CAContact: forrest@climatemodeling.org

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Strong drying conditions in the Asia-Pacific region and tropical South America during El Niño–Southern Oscillation (ENSO) lead to reduced ecosystem productivity and increased mortality and fire risk. Sea surface temperature (SST) anomalies in the equatorial Pacific drive teleconnections with temperature through changes in atmospheric circulation that also impact precipitation and soil moisture, producing indirect effects on temperature through land–atmosphere coupling. We performed a set of simulations using the U.S. Department of Energy’s Energy Exascale Earth System Model (E3SM), forced with prescribed sea surface temperatures, to study the responses and feedbacks of drought effects on terrestrial ecosystems induced by both of these events and to understand the effects of SST anomalies on temperature through changes in soil moisture. The E3SM model was configured to run with active atmosphere and land models alongside the “data” ocean and thermodynamic sea ice models. The Community Atmosphere Model used the Spectral Element dynamical core (CAM-SE) operating on the ne30 (~1°) grid, and the E3SM Land Model (ELM) was equivalent to the Community Land Model with prognostic biogeochemistry (CLM4.5-BGC). We used Optimal Interpolation SSTs (OISSTv2) and predicted SST anomalies from NCEP’s Climate Forecast System (CFSv2) as forcing. We conducted transient simulations from 1982 to present, following a spin up simulation, and analyzed the ENSO impacts on tropical terrestrial ecosystems for the 5-year periods centered on two strong ENSO events. In addition, we applied a mechanism-denial experiment to decouple the variability of soil moisture from that of SST anomalies. Soil moisture variability was found to amplify and extend the effects of SST forcing on eastern Amazon temperature and carbon fluxes in E3SM. In particular, during the dry season, after ENSO SST anomalies had dissipated, soil moisture variability became the dominant driver in the eastern Amazon, explaining 67%–82% of the temperature difference between El Niño and La Niña years, and 85%–91% of the difference in carbon fluxes. We will present simulation results and discuss the importance of capturing land-atmosphere interactions through model coupling. In addition, we will discuss the potential utility of this modeling framework for ecological forecasting on seasonal to decadal scales.

Poster #1-46**Exploring the Complex Interactions among Land Use, Vegetation Dynamics, and Hydrology in the Tropics by Incorporating Preferential Flow into FATES-ELM**

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Tropical forests play a major role in global water and carbon dynamics. Sustainable forest management by reduced impact logging and reforestation in tropical watersheds has the potential to improve the delivery of ecosystem services by improvement of water quality, increase of dry season base flow, reduction in floods, reduction in wildfire occurrence, reduction in soil erosion, and increase in carbon storage and timber production. These services depend upon the so-called *forest sponge effect*, a condition in which well-developed forest cover promotes high soil infiltrability and groundwater recharge during the wet season leading to increased streamflow during dry periods, despite the reduction in total annual runoff. Observations from tropical watersheds suggest that preferential flow (PF) is the mechanism responsible for the *sponge effect*. Preferential flow paths in soil pipes and macropores created by tree root growth and decay, soil macrofaunal burrowing, and soil shrinking/swelling significantly modulate root-zone moisture, groundwater recharge, evapotranspiration, and soil organic carbon. Preferential flow is absent in most hydrologic models and land models.

This study constitutes our first attempt to explicitly account for the influence of PF in the near-surface soil system into the FATES-ELM framework. Recent distributed hydrologic modeling studies suggest that although both lateral and vertical PF exists, the latter is more significant in magnitude and could explain the variations in streamflow patterns observed from paired catchments, where climate and substrate conditions are identical but land covers are distinct. Therefore, we have incorporated the most important feature of vertical PF by moving a fraction of water from infiltration directly to the bottom of the root zone at every time step to represent the effective contribution of PF. This fraction of quick flow is represented as a function of coarse root biomass (e.g., proportional to the mean diameter of coarse roots) that varies with land use patterns at different levels of disturbance (e.g., old-growth, clear-cut, various logging intensities), which can either be measured or calibrated depending on data availability. A set of single-point FATES-ELM simulations with and without PF will then be conducted at selected tropical sites, including Tapajos, Manaus, and Panama, and compared to observations. By using the simple parameterization of PF and improving its representation of the dynamics of water, carbon, and ecosystem demography constrained by observations, the enhanced FATES-ELM model will be a useful tool for exploring the complex interactions among land use, vegetation dynamics, and hydrology in the tropics.

Poster #1-47**Benchmarking and Parameter Sensitivity of FATES Predictions of Ecosystem Structure and Function at Barro Colorado Island, Panama**

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Projecting tropical forest dynamics and feedbacks under global change requires models that can simultaneously predict changes to ecosystem structure and function in a consistent way. The Functionally Assembled Terrestrial Ecosystem Simulator (FATES) is a dynamic vegetation model, for use in DOE's Energy Exascale Earth System Model (E3SM), developed to explore these interrelated dynamics. Here we show an assessment of model predictions of ecosystem structure (plant size distributions and functional composition) and function (ecosystem carbon, water and energy fluxes, and plant vital rates) at a testbed site in Barro Colorado Island, Panama. We compare these predictions to in situ observations and explore the sensitivity of these predictions to model parameter values as informed by plant trait observations across Panama.

Poster #1-48**First Results from the ForestGEO Hydraulic Trait Initiative**

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The ForestGEO hydraulic trait initiative seeks to understand how hydraulic traits control forest productivity and performance in a changing climate. Functional traits explain to certain degree differences in growth rates between species and ecosystems. However, commonly measured traits (e.g., wood density, leaf mass per area or leaf thickness) have limited ability to explain species' responses to water limitation. In contrary, hydraulic traits (such as turgor loss point or percentage loss of conductance) are thought to modulate tree and forest ecosystem responses to climate change. Here we present first results from a study looking at leaf turgor loss points (ψ_{tlp}) measured for species in the ForestGEO permanent forest monitoring plots on Barro Colorado Island in Panama and in the Pasoh forest reserve in Malaysia. Both forests can be classified as tropical moist lowland forest, receiving more than 2000 mm of rainfall per year. The climate in Panama is a seasonal tropical climate with a distinct dry season from January to April, whereas the climate is aseasonal in Malaysia and rainfall is evenly distributed throughout the year. Altogether, we measured ψ_{tlp} for over 120 forest tree species using the osmometric method. In Panama, ψ_{tlp} ranged between -1.25 MPa and -2.77 MPa across all sampled species and averaged at -1.65 MPa. In Malaysia ψ_{tlp} was between -1.02 MPa and -2.46 MPa and on average -1.57 MPa. Accordingly, the forest on Barro Colorado with its natural dry season has a species pool of more drought-adapted trees species than the perhumid forest at Pasoh. Both forests have tree species well adapted to drought, but they are much more common in the seasonal climate. High diversity of tree species with a large range of tree hydraulic traits is promising a certain resilience of the forest to changes in rainfall pattern with climate change. Drought will have stronger effects on the tree species composition in aseasonal forests as they contain a higher fraction of tree species with low resistance to water limitation.

Poster #1-49**Improving Hydrological and Surface Energy Fluxes by Incorporating Plant Hydraulics and Hillslope Based Drainage Function in Earth System Models**

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Spatial variability in water available for plant water use has an important control on how tropical forests respond to drought. Our previous simulations identified development needs for modeling surface and subsurface hydrology in Earth system models. First, the drought index formulation and the simplicity of treating root water uptake as a sink term in soil hydrology in the land component (ELM) of the Energy Exascale Earth System Model (E3SM) lack mechanistic representation of the interaction of soil-plant system. Second, subsurface lateral flow has been shown to have important control on surface hydrology and groundwater table depth. To address the limitation in representing hydrodynamics of the soil-plant system, we implemented in ELM the plant hydraulics scheme developed in the Functionally-Assembled Terrestrial Ecosystem Simulator (FATES). Simulations were performed at two tropical forest sites – Manaus, Brazil and Barro Colorado Island (BCI), Panama. The simulations showed that plants experience some water stress in the dry season at Manaus during the mega drought year, but the reduction in water availability is small. Combined with field characterization, simulations at BCI showed that trees experienced water stress during the 2015-16 El Niño event. We also identified the need of improvement of numerical accuracy for the plant hydraulics scheme in FATES.

To model subsurface lateral flow, we introduced a physics based representation of lateral fluxes as a drainage function using hillslopes to represent subgrid spatial variability in topography. This approach enables a realistic representation of lateral flow processes and their impacts on hydrological and surface energy fluxes, while keeping additional computational cost minimal for Earth system modeling. We coupled this model to ELM of E3SM and applied it at global scale. Simulations and analysis are used to understand (1) the role of subsurface lateral flow as a water source for river discharge; and (2) how lateral flow influences the spatial distributions of both soil moisture and water table dynamics. We will evaluate our simulations and investigate how surface heterogeneity modulates hydrological processes and the response of tropical forests to drought.

Poster #1-50**Tropical Forest Degradation Modulates Energy, Water, and Carbon Cycles in the Amazon**

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Tropical forest ecosystems are increasingly affected by human activities. In addition to deforestation, degradation from selective logging, fragmentation, defaunation, and fires alters the structure and composition of forests. Degradation impacts are concentrated at the forest frontier, with estimates that up to 70% of the forests are within 1km of forest edges. Yet, the impacts of forest degradation on ecosystem functioning remain uncertain. To better quantify and understand how changes in forest structure from degradation modulate the energy, water, and carbon cycle in Amazonian forests, we used an integrated approach that combines field and remote-sensing data with Ecosystem Demography Model (ED–2.2). We developed an algorithm to retrieve the vertical structure of forests at 50-m resolution, using a sample of 817 plots (total area = 200 ha) across the Amazon that were co-located with airborne lidar. A cross-validation analysis showed that the approach effectively captured the variability of forest structure among degraded forest classes and across regions. We then applied this method over 13,500 ha of intact and degraded forests in 5 study regions along a precipitation gradient in Eastern Amazon, to generate initial conditions for ED–2.2. First, we ran the ED–2.2 model for 3 of the study regions for which eddy covariance fluxes were available. We found that the model realistically represents the magnitude and seasonality of water fluxes and gross primary productivity, but it tends to overestimate sensible heat fluxes. In addition, we carried out 36-year (1981–2016) simulations for each of the 5 study regions, in which degraded and intact forests within each region were driven by the same meteorological drivers (MERRA–2 reanalyses and rainfall from MSWEP–2.2). Preliminary results indicated significant impact of forest structure on the seasonality of fluxes. For example, severely degraded forests showed more severe water stress and higher ground temperatures during the dry season than intact forests, and higher fire risk during mild droughts. In contrast, differences between degraded and intact forests were lower during the wet season and during extreme droughts. Our results also suggest that disturbance history sensitivity of tropical forests to drought and fire, especially during non-extreme events.

Poster #1-51**Biomass Accumulation in Second Growth Forests of Puerto Rico Using Airborne Lidar**

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Second-growth tropical forests provide important ecosystem services, such as carbon sequestration and soil stabilization. Understanding the patterns and controls of biomass accumulation in second-growth tropical forest landscapes is therefore key for advancing ecological research and earth system modeling. Here, we present an update on our efforts assessing rates and controls of second-growth forest biomass accumulation following land use abandonment across Puerto Rico. In 2017, prior to the recent catastrophic hurricanes, we surveyed the highly heterogeneous landscape dominated by second-growth forests, using a combination of field data and airborne lidar from the NASA G-LiHT imager. We estimated regrowth rates by comparison of current biomass stocks with existing detailed maps of land use history. We developed a lidar-biomass calibration model based on FIA forest inventory data. That model was applied to lidar data spread across Puerto Rico to produce biomass estimates for ~32,000 ha of forests at 26 m resolution. We developed a preliminary multivariate analysis of rates and controls of forest regrowth following land abandonment, considering gradients of soil fertility, topography, climate, and forest age. Knowledge gained from our analysis is important for improving the representation of processes controlling tropical forest carbon in Earth System Models such as E3SM-FATES.

Poster #1-52**Phosphorus Sorption to Tropical Soils with Relevance to Earth System Model Needs**

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Plant growth in many tropical soils is thought to be limited by phosphorus (P), so considering these limitations will improve predictions of vegetative productivity and global climate. Mineral soils control the availability of P because they form strong bonds with orthophosphate (PO_4^{3-}). We recently used an existing archive of 24 tropical soils and performed equilibrium batch isotherm experiments involving 0.3 g of soil and 0.03 L of solution in concentrations ranging from 0 to 500 mg $\text{PO}_4\text{-P}$ per L. The nonlinear isotherms were quantified by fitting the data to the Langmuir isotherm using the parameters Q_{max} representing the maximum sorption capacity of the soil, and K representing a binding coefficient. Our Q_{max} values ranged from 734 to 3775 mg $\text{PO}_4\text{-P}$ per kg of soil (mg/kg) with a median of 2060 mg/kg; and K ranged from 0.015 to 0.285 L/mg with a median of 0.081 L/mg. However, we have concerns as to whether the high concentrations of added P necessary to fit the Langmuir equation are realistic for tropical forest soils. Additionally, the K parameter is more sensitive than Q_{max} in the ELM model. Consequently, we modified our sorption procedure to include more low P concentrations, which results in an approximately linear isotherm at initial P concentrations < 50 mg/L. We used Puerto Rican Oxisols and Ultisols from pastures and forests to generate nonlinear Langmuir isotherms, which were then truncated in order to isolate the linear portion of the isotherm ($R^2 > 0.90$) observed at low initial P concentrations. This linear portion was used to calculate the linear distribution coefficient (Kd). Although these experiments are still in progress, the Kd thus far ranged from 18 to 432 L/kg, and the Langmuir Q_{max} ranged from 1129 to 3069 mg/kg. It is of interest to compare alternative model formulations using either the Langmuir parameters or the linear parameters, which could greatly simplify the representation of P bioavailability in soils.

Poster #1-53**Global Drivers of Vegetation Mortality**

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Tree mortality is rising in the tropics and throughout the globe, with implications on the carbon cycle and climate forcing. However, we do not yet understand the causes of this rising mortality, precluding us from mechanistic prediction under future climate. In this presentation, I will review our state-of-the-knowledge regarding the drivers and mechanisms of tree mortality with a focus on the tropics, while also extending our inference to the globe. Changes in atmospheric conditions such as rising CO₂, temperature, and VPD are plausible explanations for the global mortality rise. Mitigation mechanisms exist by which mortality may be buffered by increasing growth, but the number of mortality drivers outweighs those driving increased growth, casting doubt on the strength of the future forest carbon sink. The path forward to better understanding and simulation is highlighted.

Poster #1-54**Quantifying Forest Growth, Mortality, and Canopy Closure following Hurricane Maria**

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Hurricane Maria made landfall in Puerto Rico as a powerful, Category 4 storm. Strong winds and torrential rains snapped and uprooted trees, creating 30 to 50 times more forest gaps in one day than the island's tropical forests typically experience in a year. The loss of canopy trees altered forest structure and species composition, selecting traits that favor resilience to windthrow, and synchronized forest succession in the extensive gap area across the island. Following the storm, we remeasured long-term forest inventory plots in El Yunque National Forest and the Cambalache and Carite State Forests to quantify immediate impacts and track the rates and mechanisms of forest recovery. Here, we report results from remeasurements in paired plots with low and high damages from the storm, selected based on pre and post-storm data from NASA Goddard's Lidar, Hyperspectral, and Thermal (G-LiHT) Airborne Imager. Total mortality by species was higher from Maria than from Hurricane Hugo (Category 3). Wood density was the best predictor of total mortality by species, but not the proportion of snapped or broken trees. In addition to field surveys of mortality, branch loss, and resprouting, we installed 1000 new dendrometer bands to track stem growth for common species with differing levels of crown damage. In February, 2019, we used a Riegl VZ400i terrestrial laser scanner (TLS) to collect detailed, 3D data for each plot and complete scans of more than 200 individual trees with dendrometer bands. TLS data provide an unprecedented look at the distribution of canopy and understory vegetation to assess changes in stem density, canopy closure, and allometry from branch loss and resprouting after hurricane damages. In addition, the combination of TLS and dendrometer band data support the evaluation of diameter growth increment as a function of canopy leaf area, allocation to resprouting, and illumination conditions. Repeated TLS scans will capture dynamics of canopy closure, including the specific contributions from resprouting, regrowth, and delayed mortality for space-filling of the canopy volume over time. Tracking the structural reassembly of forests in disturbed patches will directly inform the representation of forest disturbance in FATES and other ecosystem models, including the impacts of delayed mortality and depressed productivity of damaged individuals on canopy closure and the net carbon balance of disturbed forests.

Poster #1-55**FATES Sensitivity to Forests Disturbance and Regrowth in the Amazon**

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The Landsat Ecosystem Disturbance Adaptive Processing System (LEDAPS) was developed to represent vegetation disturbance and regrowth. Whether LEDAPS is suitable to identify different disturbances and regrowth in the Amazon needs to be further examined. In this study we used LEDAPS in Landsat 5 imagery (LL5) to determine its sensitivity to spectral changes following windthrow, clearcutting, and burning in old-growth forests in Central Amazon and to assess whether the newly developed Functionally Assembled Terrestrial Ecosystem Simulator (FATES) model simulate these changes. The selected disturbances are very frequent in the Amazon and have strong influences on vegetation structure and dynamics. The results shown that all LL5 bands were sensitive to the disturbance and last from 4-6 years. Following this period, only the Near Infrared (NIR) band had significant changes associated with the disturbances and the pathways of regrowth. In general, the NIR increased with the increase in the vegetation cover, which reached its maximum after pioneers dominated the canopy and then decreased slowly and linearly to pre-disturbance conditions with the dynamics of forest succession and changes in canopy height. The faster NIR decrease rate to pre-disturbance conditions was for clearcutting, windthrow, and then burnings, respectively. After the windthrow, the NIR returned linearly to old-growth values in about 41 years in agreement with observations of biomass recovery for this type of disturbance. This in turn corroborate the sensitive of NIR to biomass changes. The NIR for clearcut and burning returned to pre- disturbance conditions after 37 and 56 years respectively. FATES predictions of biomass regrowth from windthrow and clearcut agreed with our NIR results suggesting that the dynamics of forest regrowth for these disturbances are properly represented in FATES.

Poster #1-56**Quantifying Soil Percolation Dynamics and Biogeochemical Transport in Tropical Soils near Manaus, Brazil**

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Understanding soil moisture dynamics and associated transport of biogeochemical species is challenging in tropical systems because of the physical nature of tropical soils and the coupled ecohydrological impacts on flow and transport. We utilized an unusual type of passive wick flux meter (or drainage lysimeter) to measure real-time percolation fluxes and to sample percolation chemistry and stable isotopes along two topographic transects at the ZF2 field area near Manaus, Brazil. Percolation flux is often an inferred or modeled process and as such has significant uncertainties especially in forested soils where preferential flow paths are often important. Direct measurement of fluxes provides a way to inversely calibrate hydrological model parameters which should yield more representative simulations of actual field conditions. In addition, by coupling percolation flux measurements with biogeochemistry we can understand transport dynamics of nutrients and other geochemical species. The field site is characterized by a plateau, slope, and valley type of topography, and two flux meters were installed in each of the three topographic positions. The flux meters were installed to measure the percolation flux at 60 cm below the top of the soil (which is well below the densest part of the root zone). The percolation flux results show that percolation is highly pulsed and is seasonally affected. In addition, topography is important where percolation is greatest in the valley, intermediate on the slope, and lowest on the plateau. Evapotranspiration is clearly the dominant flux relative to precipitation amounts (or throughfall), but percolation to 60 cm occurs frequently in all sites suggesting deep percolation is common even during the dry season, and that it is an important part of the site water balance. There are substantial variations in ion concentrations (e.g., calcium, sodium) through time, but the most remarkable biogeochemical behavior is associated with nitrate. Nitrate concentrations are extremely high at all locations with values sometimes exceeding 100 mg/L, and are often more than double that of chloride. Nitrate varies with topography where the slope and valley areas appear to be more pulsed, and the plateau is less variable over time. The highest concentrations were observed in the valley. These results demonstrate that nitrogen cycling is very dynamic and suggest that nitrogen is unlikely to be a co-limiting nutrient in these forests. Phosphate concentrations are frequently below the limit of detection (0.01 mg/L) although they do occasionally exceed 0.1 mg/L.

Poster #1-57**Homeostasis of Drought Tolerance Traits at the End of the Dry Season Among Trees Species at the Daintree Research Observatory in Australia**

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Tropical rainforests play a major role in biogeochemical cycles, especially carbon and water, thereby contributing to Earth's climate regulation. Climate change and especially hot drought are having negative impacts on tropical forests. We investigated the impacts of drought on tropical tree species to determine foliar turgor loss risk. To test this, we measured gas exchange (GE), non-structural carbohydrates (NSC), turgor loss point (TLP), and other traits for tree species in control versus drought treatment plots at the Daintree Research Observatory (DRO) in the Wet Tropics of Queensland Australia. Traits were first sampled in November, at the end of the dry season, and will be re-sampled in May at the end of the wet season. November-sampled data showed there were no differences in GE, NSC, or TLP between the control and drought treatments, revealing a remarkable homeostatic maintenance of traits in the face of abiotic stress. This lack of change may point to these tree species being well adapted to tolerate drought conditions. However, it may also suggest a lack of acclimation and/or plasticity. If conditions become more stressful, as is predicted by a hotter and drier future, these species may cross a threshold beyond which mortality occurs. Re-sampling of all measured traits in May will reveal seasonal effects on target traits.

Poster #1-58**Plant Hydraulic Trait Trade-offs and Species Invasion Dynamics in Moist Tropical Forests**Thomas Powell^{1*}, Charles Koven¹, Lara Kueppers^{1,2}¹ Lawrence Berkeley National Laboratory, Berkeley, CA;² University of California at Berkeley, Berkeley, CAContact: tlpowell@lbl.gov

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It has been postulated that in areas with seasonal precipitation, episodic droughts or strong soil moisture gradients, fundamental trade-offs among plant hydraulic traits are a key driver of coexistence between a diversity of plant functional types (PFTs). However, strong evidence from direct observations for such trade-offs has been elusive, which may be a consequence of sampling design and data aggregation in meta-analyses. We evaluated this assertion by using a cohort-based terrestrial biosphere model with a mechanistic representation of water transport, the Ecosystem Demography model (ED2-hydro), to explore how and where the trade-off between hydraulic efficiency and safety may emerge within a forest ecosystem. Hydraulic efficiency and safety were evaluated in terms of xylem conductivity (K_x) and vulnerability to cavitation (xylem-P50), respectively. We performed a controlled set of tropical forest simulations using local meteorological drivers and soil conditions from Barro Colorado Island, Panama and various combinations of K_x and xylem-P50. We also introduced into a mature forest at low densities an invading juvenile PFT with a hydraulic strategy differing from the native PFTs to determine both where competition governed by the efficiency vs. safety trade-off manifests itself and the conditions that allow successful invasion. ED2-hydro predicts that a strong efficiency vs. safety trade-off exists at the individual scale for trees that are in direct competition. Moreover, the K_w and xylem-P50 trait space is broad, and hence the trade-off is apparently masked when observations of numerous species within an ecosystem or biome are included without also considering the traits of the observed individual's immediate competitors. For invasions of non-native PFTs to be successful, this trade-off also depends on the developmental stage of the gaps in which the trees are growing. Invaders that germinate and become seedlings in closed-canopy patches of the forest are unsuccessful. But, invaders with superior hydraulic strategies (i.e. K_w and xylem-P50 combinations) that germinate in newly created forest gaps are successful in establishing and either coming into coexistence with the native PFTs or competitively excluding them. Therefore, our results demonstrate that this modeling framework can be used to bracket the vulnerability of forests to invaders when disturbance regimes change. We also recommend a series of new field measurements to test the hypotheses proposed by our results.

Poster #1-59**Testing for Changes in Biomass Dynamics in Large-Scale Forest Datasets**

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The response of tropical forests to ongoing climate and atmospheric changes is critical to future global carbon budgets, but remains highly uncertain. A critical question is whether increasing atmospheric CO₂ and temperature are altering forest dynamics, and if so, to what extent. Some recent studies have reported enhanced forest productivity and increased biomass stocks in old-growth forests, consistent with a fertilization hypothesis. Attribution of such increases to global change is complicated by spatial and temporal variability in biomass associated with the gap-dynamic cycle. Old-growth forests are mosaics of many small patches, with most showing small increases in biomass, and a few showing larger decreases. Hence, temporal variation in disturbances can confound detection of long-term directional change. Thus, studies of biomass dynamics must account for gap dynamics and the distribution of gap phases when testing for changes over time.

We present a new method to account for gap dynamics by analyzing biomass dynamics at the level of 10 by 10 m quadrats, analyzing quadrat-level AGB fluxes as a function of initial quadrat AGB, and evaluating whether these relationships vary over time. Using 30 years (1985-2015) of forest inventories at Barro Colorado Island (BCI), Panama, we demonstrate that AGB fluxes vary strongly with gap phase, and, despite wide inter-annual variability, found a trend in increasing productivity and mortality AGB loss over the past 15 years. Our approach points towards the importance of accounting for initial gap phase distribution in analyses of biomass dynamics, and offers to disentangle potential external forcing from disturbance-recovery dynamics.

Poster #1-60**Evaluating Leaf Photosynthesis and Stomatal Conductance Models against Diurnal and Seasonal Data from Two Contrasting Panamanian Tropical Forests**

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Tropical forests play a key role in regulating the global carbon (C), water, and energy cycles and stores, as well as influence climate through the exchanges of mass and energy with the atmosphere. However, projected changes in temperature and precipitation patterns are expected to impact the tropics and the strength of the tropical C sink, likely resulting in significant climate feedbacks. Moreover, the impact of stronger, longer, and more extensive droughts not well understood. Critical for the accurate modeling of the tropical C and water cycle in Earth System Models (ESMs) is the representation of the coupled photosynthetic and stomatal conductance processes and how environmental and other drivers impact these processes. Moreover, the parameterization and representation of these processes is an important consideration for ESM projections. We use a novel model framework, the Multi-Assumption Architecture and Testbed (MAAT), together with the open-source bioinformatics toolbox, the Predictive Ecosystem Analyzer (PEcAn), to explore the impact of the multiple mechanistic hypotheses of coupled photosynthesis and stomatal conductance as well as the additional uncertainty related to model parameterization. Our goal was to better understand how model choice and parameterization influences diurnal and seasonal modeling of leaf-level photosynthesis and stomatal conductance.

We focused on the 2016 ENSO period and starting in February, monthly measurements of diurnal photosynthesis and conductance were made on 7-9 dominant species at the two Smithsonian canopy crane sites. This benchmark dataset was used to test different representations of stomatal conductance and photosynthetic parameterizations with the MAAT model, running within PEcAn. The MAAT model allows for the easy selection of competing hypotheses to test different photosynthetic modeling approaches while PEcAn provides the ability to explore the uncertainties introduced through parameterization. We found that stomatal choice can play a large role in model-data mismatch and observational constraints can be used to reduce simulated model spread, but can also result in large model disagreements with measurements. These results will be used to help inform the modeling of photosynthesis in tropical systems for the larger ESM community.

Poster #1-61**Reconstructing Pan-Tropical Precipitation Recycling Based on Stable Isotopes**

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We used the IAEA Global Network of Isotopes in Precipitation (GNIP) database to assess the characteristics of stable isotopes (d^2H and $d^{18}O$) in precipitation at the pan-tropical scale. These data relate to tropical ecohydrology in a number of ways including moisture sources, characteristics of climate zones including seasonality and moisture recycling (e.g. local re-precipitation of water vapor derived from ET). In this study, we used monthly precipitation isotope data from 395 sites within $\pm 30^\circ$ North Latitude. We focus our efforts on investigating spatial patterns of d-excess calculated from this data due to its strong sensitivity to precipitation recycling. We employed a geospatial interpolation method to get a spatially continuous estimate of mean monthly d-excess across this latitudinal range and further classified these estimates into the three main groups of Köppen-Geiger climate zones that occur within the tropics (e.g. tropical, temperate and arid) based on differences in d-excess values. Our results show the spatial distribution of derived major Köppen-Geiger climate zones match reality in greater than 60% of the land surface at 1° resolution. Spatial matching was highest over larger continental land masses and lower where data was too sparse to appropriately resolve the interpolation as well as in regions where precipitation was more seasonally controlled. We aim to improve upon these estimates by investigating the role of specific climate and geospatial variables on d-excess values that include distance from ocean, precipitation, temperature and evapotranspiration as well as how these relationships vary seasonally. Such an effort will be useful to integrate precipitation recycling into Earth System Models (ESMs) to determine how the spatial variability of moisture sources might be changing under a warming climate.

Poster #1-62**NGEE-Tropics Data Management and Synthesis**

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The NGEE-Tropics project generates and utilizes ecological, hydrological, and meteorological datasets from tropical forests in Central and South America for scientific analysis and model parameterization and benchmarking. The goals of the Data Management and Synthesis team is to: 1) manage all project data in a community-accessible archive, and publicly release those data with appropriate citation and usage information, 2) standardize data and metadata collection for cross-site comparison, 3) curate data collected by the project and help acquire external data to create modeling testbeds, and 4) create priority data products such as meteorological model drivers, processed data with Quality Assurance/Quality Control (QA/QC), and cross-cutting synthesized datasets. The NGEE-Tropics Archive is used to internally curate and manage the project's data in preparation for public release. A public listing of all data shared publicly and with the team are available at <http://ngt-data.lbl.gov/doi>, where authenticated users can download data. In the future, NGEE-Tropics public data will be uploaded to the ESS-DIVE archive. Key data products include several rounds of QA/QC of meteorological model drivers for three sites in Panama (BCI, San Lorenzo, and Parque Metropolitano), including air temperature, relative humidity, solar radiation, barometric pressure, wind speed and wind direction. The QA/QC-ed datasets have already been used as input data for the Ecosystem Demography model (ED2-hydro) and FATES simulations. The meteorological drivers along with other project data and relevant external datasets are being assembled into testbeds to spin-up and validate model simulations. We have established collaborations with Brazil's Large-Scale Biosphere- Atmosphere Experiment in Amazonia (LBA) program to obtain high-value hydrological and micrometeorological datasets from the Amazon spanning several decades for use in NGEE- Tropics modeling efforts. Data processing of high-frequency data from the K-34 tower, and of soil moisture data in Manaus are underway. Standardized metadata reporting FRAMES templates have been used to extract critical information on sap flux measurements collected in NGEE-Tropics field sites during the 2015-2016 El Niño. This information is being used initially to synthesize data collected by different sensors in Manaus, to unify data formats and units, and to create a preliminary sap flux preprocessing QA/QC workflow. Together, the NGEE-Tropics Data Management and Synthesis objecting is focused on the long-term preservation of project data, and also create data products required to transform diverse and complex ecohydrological data into scientific understanding.

Poster #1-63**The Importance of Hydraulic Traits to Tropical Forest Dynamics**

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Vegetation plays a key role in global carbon cycles and thus is an important component within the Earth system models (ESMs) to project future climates. A recent trend for ESM vegetation modeling is to incorporate size- and succession-stage-structured demographic models. These models make it feasible for more realistic representation of key processes that control vegetation dynamics. In this study, we reported a new hydrodynamics (HYDRO) model within the DOE-sponsored the dynamic vegetation model, the functionally assembled terrestrial simulator (FATES-HYDRO). The HYDRO model is built on the size and canopy structure representation within FATES and is expected to better capture the control of hydraulic traits in both vegetation dynamics and carbon/water fluxes. In this study, we conducted a global sensitivity analysis to better understand the hydraulic trait control on tropical forest dynamics. We first assembled 10 distinct datasets of plant hydraulic traits of stomata, leaves, stems, and roots, determined the best-fit theoretical distribution for each trait, and linked these based on taxonomically-standardized species names to generate a rank correlation matrix, which quantified the degree of interspecific (between-species) trait-trait coordination. Our analysis showed that hydraulic traits that determine the soil-root connection and the stomata control are more important for dry periods, while hydraulic traits that determine the whole tree conductance are more important for wet periods. Our analysis suggests that hydraulic traits could play an important role in carbon and water fluxes and vegetation dynamics in tropical forests and further measurements to capture the hydraulic control on stomata, root-soil interface and whole tree resistance could improve our prediction of future tropical forests within ESMs.

Poster #1-64**Homeostasis of Tropical Forest Carbohydrates**

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Non-structural carbohydrates (NSCs), the organic compounds that drive plant metabolism, have rarely been studied in moist tropical forests, so their regulation in these systems is poorly understood. These compounds may modulate tree drought response and can become depleted if demand (i.e. growth, defense, respiration) exceeds supply (i.e. photosynthesis). As a result, Earth System Models (ESMs) rely on carbohydrates as a metric for vegetation survival. We measured foliar and branch NSCs of 23 canopy tree species across a large precipitation gradient in Panama during the 2015-2016 El Niño drought to examine how short- and long-term climatic variation impact carbohydrate dynamics. There was large variation in NSCs across species, however there was no change in total NSCs as the drought progressed nor across the rainfall gradient. Some NSC variation could be explained by easily and ubiquitously measured traits, providing potential for improved model benchmarking. These findings suggest that NSCs are an allocation priority in moist tropical forests and should improve our ability to capture vegetation dynamics in ESMs.

Reference:

Dickman LT, McDowell NG, Grossiord C, et al. Homeostatic maintenance of nonstructural carbohydrates during the 2015–2016 El Niño drought across a tropical forest precipitation gradient. *Plant Cell Environ.* 2018;1–10.

<https://doi.org/10.1111/pce.13501>.

Poster #1-65**Fine-Root Traits by Succession Level in Puerto Rico**

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Fine absorptive roots of vascular plants play an important role in the cycling of nutrients, carbon, and water in terrestrial ecosystems. Understanding how fine roots respond to various ecological metrics will inform model that predict how ecosystems respond to ecological stressors such as climate change. Some root traits have been shown to be highly correlated to one another, and these correlations persist when grouping tree species phylogenetically or by functional groups. This study sampled fine root vouchers from five common tree species: one native pioneer (*Cecropia scherberiana*), one introduced pioneer (*Spathodea campanulata*), one native nitrogen fixer (*Inga laurina*), and two native non-pioneers (*Dacryodes excelsa* and *Prestoea montana*). We sampled these species at six different sites in Puerto Rico with different soil phosphorus availability, plant composition, precipitation, and forest age. Only three of these species (*P. montana*, *C. scherberiana*, and *S. campanulata*) were distributed across multiple site. We measured six fine-root traits using only the first two root orders: root branching ratio, root branching intensity, root diameter, root specific length, mycorrhizal colonization, and root phosphorus concentration. We found that various root traits such as mycorrhizal colonization, specific root length, branching ratio, and phosphorus concentration showed significant relationships when grouping by successional level. Other relationships such as diameter and mycorrhizal colonization displayed trends indicating potentially similar relationships could be apparent given a larger sample size. We also found that the traits of the species that were distributed in different sites, did not change among sites. We conclude that the root traits measured in this study were related to the tree successional type and that the species that were distributed across multiple sites maintained their functional traits fixed despite the differences in forest environment.

Poster #1-66**What Drives Phosphatase Activity in Tropical Forests – A Modeling Study Using E3SM Land Model**

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Phosphorus is generally considered as the most limiting nutrient in the lowland tropical forests where soils are highly weathered with low soil phosphorus (P) availability. Most of P in tropical soils is either in organic forms or in occluded forms associated with Al and Fe oxides. Phosphatase activity, which can release phosphate from organic matter directly without carbon oxidation, provides an important pathway for sustaining P availability in tropical ecosystems. Despite its importance in providing available P, the representation of this process in models is not well constrained due to lack of measurements. Our recent field study in Puerto Rico focusing on phosphatase activity found that 1) there was an apparent inverse correlation between P availability and phosphatase activity 2) phosphatase activity varied more with tree species than with site differences in P availability due to variations in root traits. In this study our objective is to integrate the observational data with modeling in order to better understand this process and improve their representation in E3SM Land model (ELM). We first applied the ELM v1 at the three sites in Puerto Rico to evaluate the model's capability in capturing the variation in phosphatase activity between sites. We found that although the model is able to capture the inverse relationship between phosphatase activity and P availability, it overestimated the differences between the 3 sites compared with the observations. We were able to better capture the variation in phosphatase activity between sites after we improved the parameterization based on observations. We also show that by introducing root traits such as root diameters into the model, we were able to reproduce the large variation of phosphatase between species. Comprehensive sensitivity analysis has also been done to identify the most significant parameters in ELM.

Terrestrial Ecosystem Science

**Argonne National Laboratory
TES Science Focus Area**

Poster #1-34**Harmonized High-Resolution Estimates of Soil Organic Carbon Stocks and Its Uncertainties in the Permafrost Region**

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Permafrost-region soils store more than half of global soil organic carbon (SOC) stocks and are a sensitive component of the global carbon cycle under changing climate. However, our knowledge about the distribution of permafrost-region SOC stocks and their environmental controllers is limited due to the relatively sparse and uneven distribution of soil observations. As a result, substantial uncertainty exists in the current estimates of permafrost-region SOC stocks, and their fate under changing environmental conditions. Using a larger number of soil profile observations (n=2703) than previously available and spatially referenced information on environmental factors including topographic positions, land cover types, and climatic variables, we derived new high-resolution (250-m) estimates of the distribution of SOC stocks and their uncertainties (95% CI) across the northern circumpolar and Tibetan permafrost regions. In the northern circumpolar region, we estimated 510 (432–589), 441 (382–504), and 355 (311–402) Pg C are stored at depths of 0–1, 1–2, and 2–3 m, respectively. In the Tibetan region, our estimates were 9.2 (7–11), 2.5 (0.4–6), and 2.7 (1.4–3) Pg C at 0–1, 1–2, and 2–3 m depth intervals, respectively. Among topographic positions, the largest uncertainty in SOC stocks was found in the hill toe-slope positions (37%) in the circumpolar region, whereas in the Tibetan region the greatest uncertainty occurred in flat areas (63%). Among different land cover types, uncertainties in SOC stocks were greatest under needle leaved forest (69%) and lowest under wetlands (19%) in the northern circumpolar region. In the Tibetan permafrost region, we observed the largest uncertainty under grasslands (75%) and the lowest under mixed forests (10%). In the northern circumpolar region, SOC stocks decreased linearly with increasing precipitation but showed a nonlinear relationship with temperature. The uncertainty in SOC stocks increased as temperature and precipitation increased. In the Tibetan permafrost region, all relationships between SOC stocks and climatic factors were nonlinear, and in contrast to the northern circumpolar region, uncertainties decreased with increasing temperature and precipitation. We report the first harmonized assessment of SOC stocks and associated uncertainties across the permafrost domain of the northern hemisphere. Our results also provide a high-resolution assessment of permafrost region SOC stocks and their relationships with environmental factors, which can be used to optimize the collection of new field observations and benchmark the representation of permafrost-region SOC stocks in CMIP6 models.

Poster #1-35**Soil Morphology and Organic Matter Distributions of Alaskan Arctic Foothills Toposequences**

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Hillslope processes affect rates of transport, deposition, and decomposition, which impact the distribution of soil organic carbon (SOC) stocks in many regions. In the Arctic, hillslope processes and SOC stocks are further impacted by the added complexity of permafrost-affected solifluction and other lateral mass movements, cryoturbation, and patterned-ground formation. Despite increasing numbers of studies on permafrost-region SOC stocks, quantitative information across soil toposequences in the continuous permafrost zone remain limited. For instance, observations from hill-toe deposits comprise only about 2.5% of existing soil profiles for Alaska. A better understanding of soil morphology and SOC stocks across toposequences in hilly permafrost terrains is therefore critical for informing and improving future modeling efforts. In this study, two toposequences in the Arctic Foothills, north of the Brooks Range of Alaska were investigated. The soils of both toposequences were formed on loess over glacial till parent material and support moist acidic tundra vegetation. Seven locations along the toposequence (encompassing summit/shoulder, backslope/footslope, and toeslope/basin positions) were sampled by opening soil pits, taking soil cores, or a combination of both to a depth of 2-3 m. Ice-wedge polygons were present at summit/shoulder and toeslope/basin positions. Ice-wedge polygons in the basins were clearly defined, with deep inundated troughs that receive discharge from snowmelt and storms, as well as lateral discharge from thawing of the active layer and the transient layer of upper permafrost. The locations of ice-wedges at the summit/shoulder positions were less clear, but marked by surficial soil cracks, with drier troughs unless hydrologically disturbed. The thickness of surficial organic horizons was greater in the toeslope/basin positions, and some ice-wedge polygons in basins contained deep peat deposits infused with ground ice. Volumetric ice content was variable across the toposequences, most likely due to the complexity associated with patterned ground formations, such as non-sorted circles, but it was generally higher in summit/shoulder and toeslope/basin positions. Soil samples collected across the toposequences are currently being analyzed for SOC and total nitrogen concentrations. This ongoing study suggests it might be possible to uncover common patterns of soil morphology, ice contents, and organic matter distributions for arctic hillslopes but clearly underscores the need for more research on these landscapes.

Poster #1-36**Assessing the Degradation State of Soil Organic Matter in the Permafrost Region**

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The composition and potential decomposability of soil organic matter (SOM) in the permafrost region are key uncertainties in efforts to predict carbon release from thawing permafrost. The cold and often wet environment is the dominant factor limiting decomposer activity, and SOM is often preserved in a relatively undecomposed state that can be poorly associated with soil minerals. Thus, the impacts of climatic change on future SOM mineralization rates are likely to depend at least initially on the existing degradation state of SOM. Physical size fractionation is a commonly used method for characterizing and classifying the relative degradation state of peats and organic soils, with decreasing size being indicative of greater decomposition. Similarly, for mineral soils, size fractionations are used to isolate relatively undecomposed particulate organic matter (POM) from SOM that is more decomposed and/or occurs in association with soil minerals. Given that permafrost-region soils range from peats to low-carbon mineral soils and environmental conditions constrain the rate of plant residue decomposition, we are exploring size fractionation as an indicator of the relative degradation state of SOM for this region. Further, we are investigating whether the mid infrared (MIR) spectra of un-fractionated bulk soils can be used to predict the distribution of SOM among size fractions. To date, we have size-fractionated over 500 soils representing a range of vegetation types, parent materials, and genetic horizons (with <0.2 to >49% organic C) across a latitudinal transect from the Kenai Peninsula to Utqiagvik, Alaska. A large proportion of bulk SOM was found in POM pools for all soil horizon types. Even for mineral horizons, about 40% (on average) of bulk soil organic carbon occurred as POM, indicating that SOM was relatively undecomposed compared to that of typical mineral soils in more temperate regions. Analyses using a subset of these samples confirmed that the MIR spectra of bulk soils can be calibrated to reasonably predict the distribution of SOM among size fractions for permafrost-region soils. We are currently evaluating the capability of these calibrations to predict the size-distribution of SOM for the remainder of the dataset, which includes samples from independent locations. Successful development of MIR calibration models could enable widespread, high-throughput estimates of the relative degradation state of SOM stocks across the permafrost region, which are needed to benchmark and constrain local, regional, and earth system models.

Terrestrial Ecosystem Science

**Oak Ridge National Laboratory
TES Science Focus Area**

Poster #9-1**ORNL's Terrestrial Ecosystem Science – Scientific Focus Area (TES SFA): A 2019 Overview**

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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?
- 3)

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 Environment (SPRUCE) experiment testing multiple levels of warming at ambient and elevated CO₂ 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.

Poster #9-2**Peatland Vegetation Responses to 3-Years of Warming and Elevated CO₂**

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We are conducting an in situ warming by elevated CO₂ study in a high-carbon, ombrotrophic peatland in northern Minnesota. Our method to warm ten 12-m diameter plots combines a recirculating warm air envelope within enclosure walls with deep soil/peat heating to simulate a broad range of future warming treatments as much as +9 °C. Whole-ecosystem warming was initiated in August 2015, followed by elevated CO₂ atmospheres (eCO₂ at + 500 ppm) in June 2016 (half the plots). Assessments of tree growth were made with annual circumference observations at dbh, automated dendrometer band records, and annual height and canopy volume evaluations via terrestrial LIDAR. Shrub-level vegetation growth above the bog surface was obtained from destructive harvest of 0.25 m² plots in each enclosure. Sphagnum growth was measured from intact columns of selected populations. Growth data were tallied and extrapolated to the plot scale for annual estimates of plot aboveground net primary production (ANPP) for tree, shrub-layer and *Sphagnum* communities.

After three years of warming, tree growth reductions are apparent in *P. mariana* with some mortality in *Larix* evident in the warmest treatment. Shrub-layer community growth showed an increasing trend with warming, however, that community trend varied by species. No consistent growth changes driven by eCO₂ treatments for either trees or shrubs have yet developed. There was no *Sphagnum* growth response to warming or eCO₂ treatments in 2016. We observed a curvilinear response to temperature in 2017 (maximum growth for +4.5 °C plots). By 2018, a linear decline with temperature was evident. Warming reduced *Sphagnum* percent cover with declines beginning in 2016 that increased through 2017 and 2018.

Net primary production (NPP) of the *Sphagnum* community, calculated as dry matter increment times fractional cover and converted to C units, declined -13 to -29 g C m⁻² °C⁻¹ with increasing temperature in 2017 and 2018, and was less in eCO₂ plots in 2018. Shrub-layer ANPP was +3 to +4 gC m⁻² y⁻¹ °C⁻¹, and ANPP reductions for trees was -4 gC m⁻² y⁻¹ °C⁻¹. Combining all measures of ANPP shows reduced peatland C gain dominated by changes in the productivity of the *Sphagnum* layer.

Poster #9-3**The Consequences of Warming on *Sphagnum* Peat Moss Productivity and Microbial Community Composition**

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Peatland ecosystems are estimated to store a third of stored terrestrial carbon as dead organic peat. The moss plant *Sphagnum* is a keystone genus in these ecosystems, with its biological function (e.g., photosynthetic CO₂ gain, recalcitrant decomposition, acidification) and abiotic environment influencing ecosystem structure and function and potentially global C cycling. We explored the carbon and nitrogen cycling responses of *Sphagnum* to warming and CO₂ enrichment as part of the Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) project in an ombrotrophic spruce bog in the Marcell Experimental Forest in northern Minnesota. Intact plots in the bog are being exposed to a range of warming levels from ambient to ambient +9 °C in combination with ambient or elevated (900 ppm) CO₂ within 12-m diameter, open-top enclosures. The *Sphagnum* community is dominated by *Sphagnum angustifolium*, *S. fallax* (together comprising 70% cover), and *S. magellanicum* (19% cover). After one year of treatment we saw no evidence of an effect on community composition. In the second year of warming, dry matter increment of *Sphagnum* increased with modest warming to a maximum at 5°C above ambient and decreased with additional warming. *Sphagnum* cover declined from close to 100% of the ground area to less than 50% in the warmest enclosures. After three years of warming, annual productivity declined linearly with increasing temperature (13 to 29 g C m⁻² per °C warming) due to wide-spread desiccation and loss of *Sphagnum*. Productivity was less in elevated CO₂ enclosures, which we attribute to likely indirect effects of CO₂ on shrubs.

Sphagnum capitula N concentration was about 10 mg g⁻¹ in untreated plots and increased 0.5 mg g⁻¹ per degree C temperature increase. This may correspond to an increase in N availability with warming and have downstream consequences on *Sphagnum* associated N fixing symbionts (diazotroph). Therefore, we investigated the effects of warming on the microbial community and N₂ fixation activity. We found that the taxonomic diversity of the microbial community, including diazotrophs, decreased with warming (P<0.05). This was mirrored by a decrease in N₂-fixation rates. The warming treatment shifted the diazotrophs from a mixed community of *Nostocales* (Cyanobacteria) and *Rhizobiales* (Alphaproteobacteria) to those predominantly composed of *Nostocales*. Some diazotrophic genera returned to similar relative abundance as control plots after two years of warming, indicating possible taxon specific resiliency. Our results demonstrate that warming substantially alters the community composition and N₂ fixation activity of peat moss microbiomes.

Poster #9-4**Whole Ecosystem Warming Induces Divergent Ecophysiological Responses in Co-Occurring Boreal Tree and Shrub Species – Observations and Model Simulations**

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Southern boreal peatlands are considered vulnerable to projected increases in warming and the potential for environment-driven changes in seasonal patterns of net carbon uptake has strong implications for atmospheric feedbacks. At the SPRUCE whole-ecosystem warming \square CO₂ site in a Minnesota peatland, extensive interannual pretreatment gas exchange campaigns revealed significant interspecific seasonal differences in specific leaf area, nitrogen content and photosynthetic parameters (i.e., maximum rates of Rubisco carboxylation (V_{cmax25 °C}), electron transport (J_{max25 °C}) and dark respiration (R_{d25 °C})). ELM-SPRUCE was sensitive to the inclusion of observed interspecific seasonality in V_{cmax25 °C}, J_{max25 °C} and R_{d25 °C}, leading to enhancement of simulated net primary production (NPP) using seasonally dynamic parameters as compared with static parameters. Since the initiation of warming treatments, measurements at the site indicate the active season has increased by up to 10+ weeks, with sapflow beginning earlier in spring and lasting later into the fall. Warming has increased the atmospheric vapor pressure deficit and there is evidence of heat or drought-related damage in the warmest plots. Plant responses include species-specific shifts in seasonal ontogeny (developmental rates), chemistry (non-structural carbohydrates, pigments), physiology (photosynthesis, respiration) and morphology (foliar display, leaf size). The two dominant tree species displayed divergent responses to warming. In *Picea mariana*, stomatal conductance declined to reduce water loss in warmer plots, which resulted in homeostatic sapflow and leaf water potentials, and constant net photosynthesis despite increases in N content. In contrast, *Larix laricina* increased stomatal conductance and sapflow that together with increased N content led to enhanced net photosynthesis, but with dangerously low leaf water potentials. In addition, the two dominant shrub species displayed seasonally variable responses to warming and CO₂ with a wide thermal optimum for photosynthesis and differential responses of respiration. Species-specific seasonal physiological responses to warming and CO₂ treatments including shifts in the active season, ontogeny and thermal acclimation will necessitate novel model parameterization in order to improve simulation of real ecosystem-level NPP.

Poster #9-5**Warming Increases Plant-Available Nutrients in the SPRUCE Bog**

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Warming is expected to increase the release of carbon from highly-organic peatland soils, potentially leading to a positive feedback to future warming. This response is expected to be mediated by the response of peatland vegetation to rising atmospheric [CO₂], as well as the effects of warming on plant-available nutrients and water.

We quantified the effects of a range of ecosystem warming (from +0°C to +9°C), as well as elevated [CO₂], on plant-available nutrients in the SPRUCE (Spruce and Peatland Responses Under Changing Environments) experiment in an ombrotrophic bog in northern Minnesota, USA. We used ion-exchange resin capsules to monitor monthly changes in plant-available nutrients (i.e., NH₄-N, NO₃-N, and PO₄³⁻) throughout the peat profile and across hummock- hollow microtopography. NH₄-N was by far the most available N source, with NO₃-N making up a negligible fraction; PO₃⁻ availability was intermediate. Warming—combined with a longer frost-free period—tripled the availability of NH₄⁺ and PO₄³⁻ in the warmest treatment plots. Furthermore, increases in PO₄³⁻ availability with warming were greater than increases in NH₄⁺, especially in deeper peat. However, the increase in nutrients was much greater below the rooting zone. There is thus far no effect of elevated [CO₂] on nutrient availability.

Interestingly, the same warming response was not apparent in the subset of porewater nutrients collected and measured at bi-weekly intervals at a comparable depth increment in the hollows. While porewater total organic carbon concentrations were increased by warming, indicating increased mineralization of organic matter, there was no difference in porewater NH₄⁺, NO₃⁻, or PO₄³⁻ concentrations across the warmed plots.

Taken together, these lines of evidence indicate that warming has increased the mineralization of peat, leading to increased nutrient availability. In turn, increased nutrient uptake by the vegetation has depleted the availability of nutrients in the rooting zone and in porewater. The additional nutrients taken up by the plant community are detectable in increased N and P concentrations in *Sphagnum* mosses; however, this may be luxury uptake, as evidence indicates that moss production has declined with warming. The relative balance of peat accumulation will depend in part on whether vegetation growth is increased in response to warming and increased nutrient availability, or whether this response is limited by increased drying in the warmed treatments.

Poster #9-6**Genome-resolved Metagenomics Enables Fine-Resolution Assessments of SPRUCE Peatland Microbial Communities**

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Through both the direct and indirect effects of perturbation, the SPRUCE experiment is expected to lead to various alterations in peatland microbial communities and their biogeochemical processes. However, assessments of belowground communities are often challenging due to their high compositional diversity and complex functional attributes. In this effort, peat communities representing 2015 and 2016 sample collections (approx. 1 and 2 years after onset of warming respectively) were assessed with shotgun metagenomic sequencing resulting in ~1 Tbp of DNA sequence information. Through a combination of sequence assembly and binning techniques, a large proportion of the microbial community was recovered as metagenome-assembled genomes (MAGs). Our findings demonstrate that ~400 unique microbial genomes represent 70-90% of all DNA sequences recovered from intermediate and deep peat layers, and that individual MAGs are shown to exhibit strong depth-dependent abundance and gene content profiles, consistent with past studies and known physical and chemical gradients in the peat profiles. While 2015-2016 samples indicate little effect of warming on whole communities or MAG-level abundances, recent changes observed for various ecosystem properties (e.g., increased CH₄ flux, increased resin-available nutrients, and changes in plant productivity) suggest that the recently-collected microbial samples (e.g., 2017 and 2018, for which sequencing is pending) are likely to show response to experimental warming. We expect that analyses involving genome-resolved communities will enable a powerful evaluation of treatment effects on microbial composition and resulting functions. Future efforts will be able to leverage these microbial community data to track changes in MAG abundance with treatments and also in collaboration with other SPRUCE site investigators employing other 'omics methods and detailed biochemical analyses in order to model microbial physiological responses in situ.

Poster #9-7**Whole-Ecosystem Warming in a Boreal Peatland Ecosystem Alters Stream Flow and Total Organic Carbon Fluxes**

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We are investigating the effects of warming and elevated CO₂ on stream flow and solute concentrations and export as part of the SPRUCE project. SPRUCE is a large-scale, long-term experiment that is examining the effects of above and belowground warming and elevated atmospheric CO₂ concentrations on boreal peatland ecosystem processes. Ten enclosures were constructed in a black spruce-*Sphagnum* bog in northcentral Minnesota, with five temperature treatments (+0, +2.25, +4.5, +6.75, +9°C) each at ambient and elevated (+500 ppm) CO₂ concentrations. Surrounding each enclosure is a subsurface corral, and lateral outflow (i.e., stream flow) passively flows from each enclosure/corral into a collection basin for quantification. Sample collection for chemical analyses is automatic and flow-weighted using an autosampler. While a variety of solutes are measured in stream water, total organic carbon (TOC) responses are the focus of this presentation.

Stream flow, and TOC concentrations and fluxes have changed substantially with warming. Warming decreased stream flow, as cumulative annual outflow from the +9°C enclosures was 56%, 63%, and 19% lower than from the +0°C enclosures in 2016, 2017, and 2018, respectively. The effect of elevated CO₂ was less clear, but outflow tended to be lower from the elevated CO₂ enclosures. Warming has also increased TOC concentrations in stream water, but the responses were not consistent over time. In the first two years of whole-ecosystem warming, TOC concentrations were ~20 mg/L higher in the +9°C (~74 mg/L) than the +0°C (~53 mg/L) enclosures. However, in 2018, TOC concentrations were almost 50 mg/L higher in the warmer enclosures (101 mg/L vs 54 mg/L). Despite these higher TOC concentrations, annual cumulative TOC fluxes were lower from the warmer enclosures in 2016 and 2017 because fluxes were primarily driven by lower stream flow. In 2018, there appeared to be a shift in this response, as cumulative annual TOC fluxes were now higher from the +9°C than the +0°C enclosures. This suggests that the higher TOC concentrations played a larger role in driving TOC fluxes in 2018. Overall, a central focus of SPRUCE is to assess whether peatlands may shift from carbon sinks to sources under climate change. Our findings thus far suggest that TOC export from peatlands is not straightforward and will depend on whether climate change more strongly impacts the factors affecting stream flow (e.g., evapotranspiration) or TOC concentrations (e.g., peat mineralization, leaching of recently produced photosynthate).

Poster #9-8**Multi-assumption Modeling and MCMC Parameter Estimation for Testing Hypotheses of the Drivers of Seasonality in *Sphagnum* Gross Primary Production**

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Multi-assumption modeling methods allow flexible generation of many alternative models that vary in the way that processes are represented. This allows quantitative investigation of competing mechanistic hypotheses with a fuller accounting of uncertainty in parameter values and uncertainty in mechanistic understanding of the other processes in the context of ecological systems. Evaluation of alternative models must be done on a level playing field. To level the field, parameters for each alternative hypothesis should be estimated using observed datasets. In this study we develop and use advanced MCMC algorithms within the Multi-Assumption Architecture and Testbed (MAAT) to estimate parameters for alternative hypotheses (models) of drivers of the seasonality in *Sphagnum* photosynthesis. Hypotheses were investigated that describe physiological temperature responses, interactions of structure with water table height, and physiological phenology of photosynthetic traits. Parameters for these competing hypotheses were estimated against data collected using LiCOR 8100 chambers at the SPRUCE experiment sited in the S1-bog at the Marcell Experimental Forest. The optimized models (hypotheses) were then evaluated against a validation dataset from the same site collected in different years. The primary research question addressed was: what are the drivers of seasonality in *Sphagnum* GPP the primary entry point of carbon into the carbon rich peatlands of northern bogs?

MCMC based parameter estimation, optimized the fit of each hypothesis to the training data in the context of uncertainty in parameters and process representation. From this level playing field, alternative hypotheses could be used to make predictions of the seasonal dynamics in *Sphagnum* gross primary production (GPP) using environmental data from the evaluation dataset. Using AIC based goodness-of-fit of predictions to the empirically modeled GPP in these years, the best and most parsimonious hypotheses to describe seasonality in *Sphagnum* GPP were identified.

Poster #9-9**The Responses of Nitrogen and Phosphorus Cycling Dynamics to Warming and the Feedbacks to Carbon Cycling in Peatland Ecosystems**

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One of the key characteristics of peatland ecosystems is the low input of nutrients such as nitrogen (N) and phosphorus (P), particularly in bogs that receive all of their nutrients from precipitation. Primary production in peatlands has been found to be limited by N or P availability, or co-limited by both N and P. It was found that nutrient availability increased with warming in the SPRUCE warming plots. The increased nutrient availability could stimulate plant growth and lead to the indirect fertilization effect. Whether or not the peatland ecosystem carbon (C) storage will increase with warming depends on the balance between the nutrient induced indirect fertilization effect and carbon loss due to warming and drying. Here we try to explore this question through model-data integration using ELMv1-SPRUCE. We first use the pre-treatment observational data to evaluate model performance. Based on the observational data, we improve model representation and parameterization of several key processes, including soil carbon accumulation at depth and nutrient leaching. We then use the model to examine how the N and P cycling dynamics respond to warming and how the nutrient responses affect carbon cycle responses. We compare the model simulated responses with the experimental data from SPRUCE. The goal of this study is to better understand how C-nutrient interactions affect the peatland ecosystem responses to warming and to improve our predictive capability for the C-rich ecosystems in a warmer world. The model-data integration exercise will also help guide the most-needed measurements in the field.

Poster #9-10**Phenological Improvement and Evaluation of ELM Using the SPRUCE Observations**

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Phenology transitions determine the timing of changes in land surface properties (e.g., albedo and roughness) and exchanges of biosphere-atmosphere materials (e.g., carbon, energy and water). However, current phenological processes for seasonal deciduous plant types in the land component of the US Department of Energy's (DOE) Energy Exascale Earth System Model (ELM of E3SM) are based solely on growing-degree-day (onset) and photoperiod (offset) models, and are thus unable to fully characterize the long-term phenological responses under changing environmental conditions. We introduced new phenology onset and offset models to seasonal-deciduous and evergreen forests, in which the timing of plant development depends on various environmental cues (forcing and chilling processes for onset, photoperiod and air temperature for offset). The revised models were evaluated and calibrated using the unique phenology observations (e.g., the PhenoCam) in the Spruce and Peatland Responses Under Climatic and Environmental Change experiment (SPRUCE) in northern Minnesota. The impacts of using the updated phenology algorithm on major land variables were also systematically examined. We found that the revised models better represent the phenology trends responding to different warming treatments for both ambient and elevated CO₂ levels. Moreover, the earlier onset and later offset in the revised model improved the simulation of evapotranspiration and water table during the growing season. The new phenology models provide improved predictive capacity for both leaf onset and offset in mixed spruce and larch forests in the Northern Hemisphere, and more importantly, induce significant effects on the terrestrial carbon and hydrological cycles. This new modeling effort also demonstrates the potential to enhance the E3SM representation of land-atmosphere feedbacks, especially under anticipated warming conditions when chilling might be insufficient and limit the spring onset advance.

Poster #9-11**Implications of SPRUCE Results for the Long-term Carbon Balance of Boreal Peatlands: A Modeling Study Using ELM-SPRUCE**

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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. As components of complex Earth system models such as the Energy Exascale Earth System Model (E3SM), land-surface models provide crucial information about fluxes of water, energy, and greenhouse gases to the atmosphere and oceans. However, the signs and magnitudes of these fluxes depend on multiple competing feedbacks. 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. The Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment is applying whole-ecosystem warming to an ombotrophic 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, has been developed specifically to predict the experimental responses and provide a framework for eventual integration of wetland processes to Earth System models. Specifically, ELM-SPRUCE simulates hummock-hollow microtopography, bog-specific hydrology and Sphagnum moss dynamics, which were previously absent from ELM. Here we calibrate ELM-SPRUCE with observed carbon fluxes, biomass and hydrology. The calibrated model is then subjected to both experimental treatments and long-term climate change. We assess the long-term vulnerability of carbon stocks given the assumptions in ELM-SPRUCE, and the partitioning of carbon dioxide and methane fluxes. We also perform these warming simulations across a range of climates associated with boreal peatlands to place the SPRUCE results in a more regional context.

Poster #9-12**The Role of Soil Moisture on Soil Carbon Decomposition**

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Soil microbes exert complex feedbacks on soil organic carbon dynamics, which can be affected differently by changes in soil moisture and temperature. For example, soil respiration may be increased under increased temperature, but concomitant changes to microbial physiology may result in feedbacks to microbial populations that alter the carbon fluxes. However, studies of the role of soil moisture are lacking. Soils of three distinct textures (sandy, loamy and clayey) were collected from mixed forests of Georgia, Missouri and Texas, respectively, and incubated for 90 days under different moisture regimes: air dried, 25% water holding capacity (WHC), 50% WHC, 100% WHC and 100% saturation. Soil respiration was measured weekly, and destructive sampling was conducted at 1, 15, 60 and 90 days to determine microbial biomass carbon and nitrogen, dissolved organic carbon, and hydrolytic enzyme activities. Results showed that CO₂ production is higher in clayey soil followed by loamy and sandy soils. Sandy soils have the highest CO₂ efflux at 50% WHC, loamy soils at 100% WHC, and clayey soils at 100% saturation. In general, microbial respiration exhibits a bell-shaped response to moisture variation regardless of soil texture, while hydrolytic enzyme activities increase with increasing moisture content. We extended the experimental results by conducting a theoretical analysis of the response of microbially-mediated SOC decomposition to intensified soil moisture extremes by the end of the 21st century at the Missouri Ozarks AmeriFlux (MOFLUX) site, using our Microbial-ENzyme Decomposition (MEND) model. The magnitude of microbial respiration reduced by drought is greater than that of increased microbial respiration by wetting. Under extreme drought, all active microbial biomass, enzyme activity and turnover rates of SOC pools decreased more compared to wetting, resulting in lower cumulative soil C loss under intensified moisture extremes. These findings remain true even when the effect of changing inputs, i.e., changes in substrate supply, are considered. Both the experimental and modeling studies emphasize the nonlinear response of soil microbial response to moisture variations. Currently, most soil carbon studies are focused on temperature responses, while this work points to the importance of the sensitivity of SOC dynamics to soil moisture.

Poster #9-13**Sun-induced Chlorophyll Fluorescence and Its Importance for Modeling Photosynthesis from the Side of Light Reactions**

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Recent progress in the observation of sun-induced chlorophyll fluorescence (SIF) provides an unprecedented opportunity to advance photosynthesis research in natural environments. However, we still lack an analytical framework to guide SIF studies and integration with the well-developed active fluorescence approaches. Here we present this framework. We derive a set of coupled fundamental equations to describe the dynamics of SIF and its relationship with C₃ and C₄ photosynthesis. We show that SIF is dynamically as complex as photosynthesis. However, the measured SIF simplifies photosynthetic modeling from the side of light reactions because it integrates over the dynamic complexities of photosynthesis. Specifically, the measured SIF contains direct information about the actual electron transport from photosystem II to photosystem I, giving a quantifiable link between light and dark reactions. With much-reduced requirements on inputs and parameters, the light reactions-centric, SIF-based model complements the traditional, dark reactions-centric biochemical model of photosynthesis. The SIF-photosynthesis relationship, however, is nonlinear because photosynthesis saturates at high light while SIF has a stronger tendency to keep increasing as fluorescence quantum yield is relatively insensitive to light levels. Successful applications of the SIF-based model of photosynthesis will depend on predictive understanding of the dynamics of fraction of open photosystem II reaction centers, canopy escape probability of SIF photons, stomatal and mesophyll conductance, etc. Advances can be facilitated by coordinated efforts in plant physiology, remote sensing, and eddy covariance flux observations.

Poster #9-14**Temperature Response of Foliar Dark Respiration and Consequences for the Stand Carbon Budget**

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Understanding the temperature response of photosynthesis and foliar dark respiration (R_d) is needed in formulating hypotheses about vegetation response to climate change. Proper representation of temperature response is also required of models used to predict these responses. Accordingly, we are evaluating alternative model formulations of leaf-level temperature responses of photosynthesis and R_d and their consequences for simulated carbon fluxes at the leaf, canopy, and stand levels. Here we report results for modeled temperature response of foliar R_d . We first compared simulated leaf-level R_d temperature response curves from nine alternative formulations with pre-treatment observations of black spruce (*Picea mariana*) at the SPRUCE (Spruce and Peatland Responses Under Changing Environments) experimental site in northern Minnesota. We found divergence across models at temperatures greater than 35°C, but the models as a group matched the observed temperature response below $\approx 30^\circ\text{C}$. We next integrated the different temperature-response functions into the ELM-SPRUCE model as alternative formulations for leaf maintenance respiration $R_{m,\text{leaf}}$ and simulated stand-level carbon flux across pre-treatment years 2011-2015. We found that the various formulations made little difference in simulated $R_{m,\text{leaf}}$, canopy maintenance respiration $R_{m,\text{canopy}}$, autotrophic respiration R_a , net primary production NPP or net ecosystem production NEP, largely because temperature was usually in the range over which the response functions are most similar and rarely exceeded 30°C. We next examined the impact of the alternative formulations on model response to the SPRUCE experimental treatments of +0.00, +2.25, +4.50, +6.75 and +9.00°C. In these simulations air temperature can exceed 35°C and differences in leaf-level temperature response became apparent in $R_{m,\text{canopy}}$, R_a , NPP and NEP. There was, however, a general narrowing of the differences when moving from the leaf to the stand. Effects of the different respiratory temperature-response formulations on five-year mean annual NEP at +9.0°C ranged from -10 to 3%. With formulations representing acclimation, simulated net carbon loss was reduced by $\approx 20\%$ in some years. Choice of foliar R_d temperature response function can substantially affect simulated stand's carbon budget.

Poster #9-15**A Multiscale, Multifidelity Land Model Testbed Assisted by Machine Learning**Dan Lu¹, Daniel Ricciuto¹, and Dali Wang^{1*}¹ Oak Ridge National Laboratory, Oak Ridge, TNContact: wangd@ornl.gov

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We propose to use artificial intelligence (AI) technologies to design a dynamic testing, uncertainty quantification (UQ) and development platform for the above ecosystem functions within E3SM Land Model (ELM). This flexible testing platform may take as inputs either ELM- generated drivers or measurable external forcings at experimental sites and will generate spatial- temporal driving data for specific ecosystem functions. This will dramatically reduce the data dependency to generate standalone functional units for further ecosystem experimental design, testing of new algorithms, UQ or module-based integration. Model development may be done within these units, allowing for more efficient coding, simulation and evaluation. These standalone units, if sampled sufficiently over the possible space of parameters and drivers, can also be substituted by AI-based surrogate models. These AI-based surrogate models demonstrate greatly improved accuracy over traditional surrogate approaches (Lu et al., 2019). Model parameter calibration (e.g. Lu et al., 2018) and sensitivity analysis (e.g. Griffiths et al., 2017) will be performed using these surrogate models. Model development focused on a specific submodel (e.g. carbon allocation) can use the surrogate representations of other expensive submodels (e.g. GPP), allowing the model developer to understand the feedbacks within the full land model in the context of uncertainty while retaining the ability for rapid evaluation. The surrogate representations will necessarily have some loss of fidelity, but we expect to minimize this loss through improved neural network training capabilities on HPC and new algorithms. In addition, we will exploit multifidelity techniques such as multi-level monte carlo to perform uncertainty propagation while considering multiple model structures.

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Poster #9-16**Advancing Predictive Understanding of Terrestrial Ecosystem through Machine Learning**Dan Lu^{1*} and Daniel Ricciuto¹¹ Oak Ridge National Laboratory, Oak Ridge, TNContact: lud1@ornl.gov

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

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

Improving predictive understanding of terrestrial ecosystem variability and change requires data- model integration. Efficient data-model integration for complex models requires surrogate modeling to reduce model evaluation time. However, building a surrogate of a large-scale terrestrial ecosystem model (TEM) with many output variables is computationally intensive because it involves a large number of expensive TEM simulations. In this effort, we propose an efficient surrogate method capable of using a few TEM runs to build an accurate and fast-to- evaluate surrogate system of model outputs over large spatial and temporal domains. We first use singular value decomposition to reduce the output dimensions, and then use Bayesian optimization techniques to generate an accurate neural network surrogate model based on limited TEM simulation samples. Our machine learning based surrogate methods can build and evaluate a large surrogate system of many variables quickly. Thus, whenever the quantities of interest change such as a different objective function, a new site, and a longer simulation time, we can simply extract the information of interest from the surrogate system without rebuilding new surrogates, which significantly saves computational efforts. We apply the proposed method to a regional TEM to approximate the relationship between 8 model parameters and 42660 carbon flux outputs. Results indicate that using only 20 model simulations, we can build an accurate surrogate system of the 42660 variables, where the consistency between surrogate prediction and actual model simulation is 0.93 and the mean squared error is 0.02. This highly-accurate and fast-to-evaluate surrogate system will greatly enhance computational efficiency in data-model integration to improve predictions and advance our understanding of terrestrial ecosystems.

Publication

Lu, D. and Ricciuto, D.: Efficient surrogate modeling methods for large-scale Earth system models based on machine learning techniques, *Geosci. Model Dev. Discuss.*, <https://doi.org/10.5194/gmd-2018-327>, in review, 2019.

Poster #9-17**Short- and Long-Term Dynamics of Leaf, Wood, and Fine-Root Production at the ORNL FACE Site**Yao Liu^{1*}, Anthony P. Walker¹, Colleen M. Iversen¹, and Richard J Norby¹¹ Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TNContact: liuy6@ornl.gov

BER Program: TES

Project: FACE Model Data Synthesis

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

The major components of a woody plant (leaves, wood [stem and coarse root], and fine roots) are produced under different phenological cycles, which could influence ecosystem carbon, nutrient, and water cycling. However, current understanding of leaf, wood, and root dynamics are generally developed in isolation because studies rarely measure production of these components simultaneously, especially at sub-annual time steps. The interplay among different tissue types at the intra-annual scale, therefore, remains largely unknown. One of the benefits of DOE BER funding of long-term experiments has been the multi-year focus on the components of net primary production, and their response to environmental change. To address the knowledge gap, we assess leaf, wood, and fine-root production at monthly and finer time steps from the intensively studied Oak Ridge National Laboratory (ORNL) Free-Air CO₂ Enrichment (FACE) site. For each tissue type, we quantify a number of important phenophases that have been previously identified in the literature, including the start, end, peak, duration, and lead-lag between different tissue types. A multivariate statistical model of production dynamics is developed to address three questions: (i) How is phenology of different components related? (ii) To what extent is the timing of production influenced by environmental drivers (daylength, temperature, precipitation, soil water and temperature, CO₂) versus the production of other tissues (i.e., exogenous compared with endogenous control)? (iii) How is production phenology related to annual production in a given year?

The phenology of leaf, wood, and fine-root production for *Liquidambar styraciflua* at the FACE site was revealed: among the three components, leaves have the shortest production season, which is constrained to the spring as expected; the peak of wood production coincides with the end of leaf production, and in some years, a small fraction of wood is produced before leaf expansion; fine root is generally produced in two phases, including a pulse in the early spring that precedes leaf expansion and a more uniform production that follows wood production and lasts into late fall. We found that production phenology varied more across years than among treatment rings and between CO₂ treatments. We aim to use this empirical groundwork as a foundation to guide the representation of intra-annual production dynamics in ecosystem models, as well as to stimulate new hypotheses and analyses to better understand the dynamic, co-varying components of woody plant growth.

Terrestrial Ecosystem Science

**Lawrence Berkeley National Laboratory
TES Science Focus Area**

Poster #9-21**The Berkeley Lab Terrestrial Ecosystem Science SFA on Belowground Biogeochemistry: Five Years of Deep Soil Warming**

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BER Program: TES

Project: Berkeley Lab TES SFA on Belowground Biogeochemistry

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

In the Berkeley Lab Terrestrial Ecosystem Science SFA, we conduct basic research on 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 next-generation predictive capacity suitable for Earth system models. Current SFA research is centered around a set of field, laboratory, and model experiments to characterize how biotic and abiotic processes influence soil carbon cycling, and how they may shape ecosystem responses to a warming climate. We are conducting a field experiment in a well-drained coniferous forest in which we are warming the whole soil profile (+4°C) and adding ¹³C-labelled litter at different soil depths. We are using the experiments to evaluate the influence of soil depth, mineralogy, biota, and climate on soil carbon dynamics, and applying the results and observations to inform model structures and parameters. We are using experimental data from the deep soil warming, incubations, and other studies to guide model development in a reactive transport framework (BeTR; Tang et al. 2013), and integrating this into the DOE E3SM land model (ELM). This poster will present biogeochemistry results from the Blodgett Forest whole soil warming experiment over its first five years. Research on microbiology, mineralogy, and modeling are in posters by Alves, Nico, and Lyu respectively.

During the first two years of the experiment, warming increased CO₂ respiration by 35% (Hicks Pries et al. 2016). After five years of warming (spanning both wet and drought years), soil respiration averaged 30% higher compared to the control plots with no trend in the effect size. During some of the hot, very dry summer months however, the warmed plots had lower soil respiration than the controls (a negative warming response). Warming also increased the amount of dissolved organic matter in both shallow and sub-soils, but in surface soils this effect decreased over time. In contrast, there was no effect of warming on dissolved nitrogen in the soil leachate. Our soil respiration and leachate data over five years of whole-soil warming suggest that CO₂, dissolved organic carbon, and dissolved nitrogen, and their response to warming, are decoupled over time and with depth.

Hicks Pries, C.E., C. Castanha, R. Porras, and M.S. Torn. 2017. The whole soil carbon flux in response to warming. *Science* 2017; eaal1319 DOI: 10.1126/science.aal1319

Poster #9-22**The Role of Microbial Traits in the Response of Soil Respiration to Warming Through the Soil Profile in the LBNL TES SFA**

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BER Program: TES

Project: Berkeley Lab Terrestrial Ecosystem Science SFA on Belowground Biogeochemistry

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

The mechanisms and responses of soil organic matter (SOM) decomposition to warming remain some of the largest uncertainties in ecosystem-climate feedbacks. Moreover, current knowledge of these processes is mostly limited to surface soils, although over 50% of global soil carbon is contained in sub-soils below 30 cm. Soil physicochemical conditions, nutrient inputs, and organic matter chemistry change with soil depth, partly due to a decreasing influence of plant inputs and root-microbe interactions. Such factors select for microbial communities with distinct metabolic, physiological, and cellular properties (i.e., microbial traits) that may constrain SOM decomposition, and the trajectory and magnitude of the respiration response to warming through the soil profile.

In the LBNL TES SFA, we are investigating microbial responses and feedbacks to warming through the whole soil profile using continuous field-based warming experiments at temperate forest and grassland sites, and complementary short- to mid-term laboratory manipulations. We have previously observed that surface and sub-soils at the forest site harbor consistently distinct bacterial communities and that in situ warming over 18-30 months induced transient changes in both community composition and carbon use efficiency (CUE; determined based on substrate-specific metabolic modeling). This led us to hypothesize that the emergent soil respiration response to warming is largely driven by the interplay between selection of microbiomes with distinct metabolic and physiological traits through the soil profile, and their responses to varying environmental conditions.

In the current phase, we are: (i) investigating the dynamics of genome-derived functional and evolutionary traits (based on metagenomic analyses) through the soil profile, and their relationships with soil properties that co-vary with depth and environmental factors, including warming; (ii) implementing new stable isotope-based and substrate-independent methods to quantify microbial population growth rates, turnover, CUE, and nitrogen transformations; (iii) using laboratory incubations to infer generalizable, mechanistic relationships between microbial traits and critical environmental factors (substrate quality, and nutrient and water availability); and (iv) parameterizing microbial processes in soil biogeochemical models using microbial traits and leveraging laboratory experiments to benchmark models to scale short-term mechanisms to longer-term field observations. Initial results from laboratory experiments suggest that respiration in both surface and sub-soils is co-limited by carbon and at least nitrogen or phosphorus, and that warmed surface soils (after 5 years) are relatively more carbon limited than unwarmed surface and sub-soils. To elucidate interaction mechanisms between microbial physiology, nutrient availability and warming, we are currently quantifying gross microbial growth, turnover, and CUE.

Poster #9-23**Temperature and Soil Moisture Impacts on Decomposition of Mineral-Associated Carbon: LBNL TES SFA**Peter S. Nico^{1*}, Rachel Porras¹, and Margaret S. Torn¹¹ Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, CAContact: psnico@lbl.gov

BER Program: TES

Project: LBNL TES SFA on Belowground Biogeochemistry

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

Soils are an important reservoir of organic carbon (OC) in the global carbon cycle. It is well established that interactions with minerals are one of the primary mechanisms by which otherwise decomposable carbon accumulates and is retained in soils and sediments. However, the bioavailability of different mineral-associated organic substrates under varying environmental conditions is not well understood. Previous work under this SFA found there was a dramatic decrease in the decomposition of glucose, an otherwise highly decomposable organic substrate, when it was adsorbed to synthetic goethite and ferrihydrite. Specifically, association with Fe (hydr)oxide minerals reduced decomposition of added glucose by over 95%. Although absolute respiration rates of native OC were much lower in the deeper soils, respiration rates normalized by total OC did not differ from surface rates, implying that total carbon availability limits respiration at depth. Following further analysis, we found that the temperature sensitivity of total respiration (native C and glucose) appears to be greater in the deeper soils but sensitivity of mineral-associated organic carbon appears to be less sensitive than native carbon. To assess the impact of temperature and moisture on the decomposability of mineral-associated glucose in soil, we conducted a series of laboratory incubations at two different temperatures (25 °C and 30 °C) and two different moisture levels (20% VMC and 30% VMC) with field- collected soils from two depths (10-20 cm and 80-90 cm). ¹³C-labeled glucose was added either directly to the soil or after it was adsorbed to with poorly crystalline synthetic iron (hydr)oxide (ferrihydrite). While temperature and moisture enhanced decomposition rates, the effect was more pronounced for native OC than for mineral-associated glucose and greater in surface soils.

Our results show how the changing moisture and temperature regime within a soil affect the sorption-desorption behavior of an otherwise readily metabolized organic substrate and how these moisture- and temperature-induced responses vary with depth.

Poster #9-24**A Site- to Global-Scale Soil Biogeochemical Model in ELM with Vertically-Resolved Microbe- and Mineral-Surface Representations: Application to the LBNL TES SFA Warming Experiment**

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BER Program: TES

Project: LBNL TES SFA on Belowground Biogeochemistry

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

Accurately predicting soil carbon responses to a changing climate is difficult, and has been limited by the lack of long-term soil warming experimental observations that can be used to develop and test mechanistically based soil biogeochemical (BGC) models. Most soil BGC models simulate soil organic matter dynamics based on decay rates of conceptually defined organic matter pools. They lack explicit description of interactions among components actively involved in soil reactions, which are influenced by environmental factors such as temperature and moisture. The lack of explicit reaction processes can result in unrealistic BGC responses to both sudden and gradual changes in environmental drivers. To provide more realistic simulations of dynamic soil physical, chemical, and biological processes—and thus of the soil response to environmental change—we have developed a model in ELM-BeTR that explicitly represents microbial physiology and their interactions with soil minerals, substrates, and plants. We applied the newly developed model to the deep soil-warming experiment at Blodgett forest in northern California with the goal to reproduce the observed soil biogeochemical responses to multi-year warming. Our preliminary results indicate a good comparison with vertical profiles of soil organic matter content and CO₂. The new model will contribute to a more comprehensive and realistic terrestrial ecosystem model that can be applied to site and global simulations.

Terrestrial Ecosystem Science

Pacific Northwest National Laboratory Soil Biogeochemistry Study

Poster #9-29**Pore- to Core-Scale Controls on Ecosystem CO₂ fluxes: Water Dynamics Drive the Microbial Cycling of Soil Carbon**

Vanessa Bailey,^{1*} Peyton Smith,¹ Taniya Roy Chowdhury,² Sarah Fansler,¹ Jianqiu Zheng,¹ and Ben Bond-Lamberty³

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BER Program: TES

Project: PNNL Project

Soil structure and water combine to regulate soil organic carbon and nutrient bioavailability, which in turn drive microbial activities. The physical structure of soil constitutes both the flow paths for resource transport in the aqueous phase and the habitat for soil microbes. The soil water is both the solution for solute transport and the reagent within which biogeochemical transformations occur. When soil moisture decreases, the hydrologic connectivity between soil pores decreases, and the concentrations of solutes in the remaining soil waters increases. The objective of this research was to measure the effect of drought vs saturation on the mobilization of soil C through the soil pore network, on the forms of soil C in the soil pore network, and on the C cycling activities of the soil microbial community. We used soils from Alaska, Washington, and Florida to test three hypotheses: i) Soils that have been subjected to a simulated drought will have greater proportions of complex C species, and microbial communities will experience local osmotic stress. ii) Soils that have been subjected to extended saturation will have a greater proportion of simpler C, and the soil microbial communities will be able to move through the hydrologic connections to access soil C. iii) Soils that were held at field-moist conditions will reflect the resource islands that occur as a result of discontinuous water connections and the relative diversity of C molecules, microbial functions, and taxa will be highest in these soils. We combine advanced techniques for molecular characterization of soil C with tomography to reveal where in the soil matrix SOC persists, and in what forms. We imposed extreme water conditions, from drought through flood, and found that moisture history matters a great deal to the forms of C in soil, where they are located, and how they contribute to CO₂ emitted through heterotrophic respiration. Each soil responded differently to the extreme water conditions, however these differing responses may be attributed to fundamental differences in the abundance of fine pores in each soil.

Poster #9-30**Soil Moisture Control on the Temporal Scaling and Prediction of Soil Respiration**

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Project: PNNL

Understanding the temporal variability and dependencies of carbon fluxes is critical to robustly scaling individual measurements across time and space. In particular, soil respiration (R_S), the soil-to-atmosphere CO_2 flux that originates from both heterotrophic and autotrophic sources, is a key component of the carbon cycle but difficult to predict. R_S at collar- to ecosystem- scales is controlled by a complex cascade of biotic and abiotic processes, and soil moisture has emerged as a key but complex factor: in conjunction with soil structure it regulates soil organic carbon and nutrient bioavailability, driving microbial activities, but its importance varies across temporal and spatial scales. We examined the degree to which R_S at long timescales can be predicted by its flux at mean annual temperature, an idea first advanced by Bahn et al. (2010), and how this relationship varies under different soil moisture regimes and in long-disturbances such as drought. Monthly and annual databases of measured R_S flux are used to test the robustness, accuracy, and bias of the Bahn scaling under different soil moisture (as well as other abiotic and biotic) conditions. These results can also be linked to pore-to-core scale analyses that examine the laboratory sensitivity of heterotrophic respiration to imposed drought and rewetting conditions. Because R_S cannot be measured over large spatial scales, and over continuous temporal scales only to a very limited extent, robust scaling mechanisms are the key to credible gap filling, as well as producing the wall-to-wall data products necessary for global flux assessments and earth system model benchmarking.

Poster #9-31**Pore- to Core- Controls on Ecosystem CO₂ fluxes: Soil Microscale Hydrology Drives Thermodynamic Controls on Carbon Decomposition**Jianqiu Zheng^{1*}, Ben Bond-Lamberty², Vanessa L. Bailey¹¹ Pacific Northwest National Laboratory, Richland, WA² Joint Global Change Research Institute-Pacific Northwest National Laboratory, College Park, MDContact: jianqiu.zheng@pnnl.gov

BER Program: TES

Project: PNNL Project

Developing models that accurately simulate soil processes is an important challenge in predicting soil organic carbon decomposition and projecting atmospheric carbon dioxide concentration in response to environmental changes. Microbial-explicit biogeochemical models are rapidly developing and significant efforts have been put into microscale characterization of microbial functions, and harmonization of microbial models with observations. Yet the incorporation of microscale soil physical structure and hydrology has lagged behind the numerical representation of soil microbial dynamics. Soil water influences the physicochemical habitat for microbes that drive soil carbon cycling by regulating the availability and transport of carbon and other nutrients, but microbially-explicit responses to soil moisture changes and associated physicochemical changes are largely missing. Here we leverage our previous observations on how soil moisture regulates carbon decomposition in different soil types to represent the relationship between soil hydro-geochemistry and carbon decomposition in a microbially- explicit model. In particular, we attempt to incorporate the influences of soil physical structure and pore networks on organo-mineral interactions, microbial growth kinetics and enzymatic functions. To account for these controls, we built a microbially-explicit carbon decomposition model into a geochemical framework PHREEQC, which allows aqueous chemistry and thermodynamic calculations. Through modeling carbon decomposition under varying soil moistures within distinct soil types, we demonstrate that parameterization with one pre-selected moisture response function generates significant uncertainties. We further employ a new moisture function that considers variations in soil properties by introducing competitive diffusion of organic carbon and oxygen, and the collocation of organic carbon and microbes. This new moisture function addresses part of model uncertainties by providing more flexibility in representing moisture responses. Investigation of microbial explicit responses to soil moisture changes and associated physicochemical environmental changes is needed to further resolve model uncertainties in predicting carbon cycling in response to soil moisture.

Terrestrial Ecosystem Science

**Lawrence Berkeley National Laboratory
AmeriFlux Management Project**

Poster #9-38**The AmeriFlux Management Project: Overview and the Year of Methane**

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Project: AmeriFlux Management Project

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

AmeriFlux is a network of sites and scientists measuring ecosystem carbon, water, and energy fluxes across the Americas using eddy covariance techniques. The DOE AmeriFlux Management Project (AMP) works to enhance the value of AmeriFlux for Earth system modeling, terrestrial ecosystem ecology, remote sensing, and many other fields. In February 2019, AmeriFlux registered its 400th site, three times the number of sites in 2012, and more than 75 of these measure methane fluxes. AMP is supporting operations of 14 clusters of long-term flux sites, maintaining the continuity of valuable time series. The connection with NSF's National Ecological Observatory Network (NEON) is bearing fruit, with 30 NEON sites now registered in AmeriFlux and seamless data cooperation between the networks. AMP has teams dedicated to four tasks: Technical support and QA/QC, Data support and QA/QC, Outreach, and Core site support. This poster highlights our first-ever theme for network action, The Year of Methane. See AMP posters by Christianson and Pastorello on data processing and products; Biraud on the Rapid Response loaner system; and Chu on a footprint analysis tool under development.

The Year of Methane! AmeriFlux launched its first theme year for network action, centered on this important greenhouse gas, at an AGU Town Hall and the AmeriFlux PI Meeting. Through outreach, data, and tech activities, the theme year will enhance the quality and impact of methane flux measurements. (1) To promote community interaction we launched a new website for news, blogs, and events. In the next year we will hold a community workshop on Methane fluxes to encourage best-practices and data synthesis. (2) For technical resources, we are providing loaners of two fast-response methane sensors. We are measuring methane fluxes as part of the Tech- team site visits and providing CH₄ calibration gases to active sites. (3) To support methane-data processing and sharing, we have added new variables like water temperature to the standard file formats, and will assist with online data access curated by the Global Carbon Project FLUXNET Methane Synthesis project. We are partnering with the Global Carbon Project, Coastal Carbon RCN, Europe's RINGO project, and others. The initiative is already leading to new sites in methane producing ecosystems and publishing new data on methane fluxes. Join the AmeriFlux Year of Methane community at ameriflux.lbl.gov/year-of-methane.

Poster #9-39**The AmeriFlux Rapid Response System**

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Project: AmeriFlux Management Project

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

The AmeriFlux Management Project has three Rapid Response flux systems that we loan to scientists to take advantage of unique research opportunities that arise quickly, or may have short measurement windows. Such situations might include: measuring ecosystem fluxes following a disturbance, such as a wildfire, an infestation of borer beetles, or a habitat restoration.

Researchers may need to quickly start useful measurements of ecosystem response and recovery. They might plan to make measurements just for a short time or they may plan to seek funding to purchase a system for long-term measurements and use the Rapid Response flux system to fill the gap in time until that process is successful.

In this poster, we present preliminary results from two deployments of Rapid Response systems following:

- A wildfire disturbance in New Mexico that burned the Valles Calera National Preserve in May 2013, where two AmeriFlux sites were established in 2006 in ponderosa pine forest and subalpine mixed conifer forest. These sites are the two highest elevation sites in the New Mexico Elevation Gradient (NMEG) study led by Marcy Litvak. The Ponderosa pine site did not burn, but the mixed conifer forest experienced a stand-replacing fire. The rapid response system deployment enabled monitoring of short-term changes in carbon, water, and energy fluxes immediately following the burn and quantification of how these fluxes change as the forest recovers.
- A plant species composition change that is underway in Florida coastal wetlands, where mangroves are invading coastal wetlands. A flux tower system was setup in a *Spartina* and *Juncus* marsh (no mangroves yet) in 2017 as part of this study. A Rapid Response system was installed in late 2017 into a mangrove-invaded *Spartina* Marsh (US-KS4). The pair of flux towers could provide answers to changes caused by the “lignification of graminoid marshes”.

Poster #9-40**Scaling AmeriFlux Data Activities to Support Network Growth**

Danielle S. Christianson^{1*}, You-Wei Cheah¹, Housen Chu¹, Gilberto Pastorello¹, Fianna O'Brien¹, Yeongshnn Ong¹, Dario Papale², Makayla Shepherd¹, Marty Humphrey³, Deb A. Agarwal¹, and Margaret S. Torn¹

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Project: AmeriFlux Management Project

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The AmeriFlux Management Project (AMP) Data Team offers diverse data services to AmeriFlux flux-tower teams and data users including: high-frequency data storage, QA/QC processing, DOIs, and standardization of flux and meteorological (flux-met) data. The network has over 400 sites, with more than 200 actively contributing data. In this poster, we highlight efforts to meet increasing demand for AmeriFlux data services, primarily QA/QC processing of flux-met data and supporting Biological, Ancillary, Biological, and Metadata (BADM).

Providing standardized, QA/QC'd flux-met data to the Earth science community is a core data service. The AmeriFlux BASE data-processing pipeline accepts flux-met data in a standardized half-hourly submission format (called FP-In). Automated QA/QC checks are performed and results are communicated with flux-tower teams via on-line reports and a customized issue tracking system. After successfully passing the QA/QC assessment, data are downloadable from the AmeriFlux website as the AmeriFlux BASE data product. We continue to add automation to the data-processing pipeline, including same-day online preliminary feedback to flux-tower teams. Teams can further track their site's data-processing status via a tool on at ameriflux.lblo.gov. In addition, the BASE product follows the FP-Standard format, which significantly expands the number and types of variables included in data submissions and products. Data users will soon be able to search over 1750 sites years (from over 250 sites) of BASE data by variable name and year on the updated AmeriFlux Site Search webpage. New figures summarizing the data are also in progress. The AmeriFlux BASE data product is processed further, including gap-filling and flux partitioning, by ONEFlux, the next generation of FLUXNET processing (see poster by Pastorello et al.).

The BADM templates, used to organize and share non-flux data from tower sites, continue to evolve. The BADM Web interface allows flux-tower teams to easily submit or update site general information BADM. The new Variable Information online tool has been used by over 75 tower-teams to provide height and instrument-model information that is shared via the new Measurement Height data product. We are upgrading the 15-year-old BADM infrastructure to enable QA/QC processing of BADM similar to flux-met data. As part of this process, we are developing new submission interfaces collaboratively with flux-tower teams. The AmeriFlux data team continually works to improve the flux-tower team and user experience and to increase the breadth, quantity, and quality of AmeriFlux data available for synthesis and analysis to address today's science challenges.

Poster #9-41**New AmeriFlux data products using the ONEFlux pipeline**

Gilberto Z. Pastorello^{1*}, Danielle S. Christianson¹, Housen Chu¹, You-Wei Cheah¹, Abdelrahman Elbashandy¹, Fianna O'Brien¹, Makayla Shepherd¹, Carlo Trotta², Eleonora Canfora², Dario Papale², Dennis D. Baldocchi³, Sebastien C. Biraud¹, Deb A. Agarwal¹, and Margaret S. Torn¹

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BER Program: TES

Project: AmeriFlux Management Project

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

The data products for AmeriFlux are being continuously improved and expanded. The AmeriFlux BASE product – the flux and meteorological data product – now benefits from extended quality control protocols that identify and address potential data issues sooner. We are also now collecting more detailed instrument and variable information, allowing more precise interpretation of the data. These products rely on increased automation, allowing faster publication of AmeriFlux data. For more information on these and other products, see the Christianson et al. AmeriFlux poster.

Another important development for AmeriFlux data products is the ONEFlux pipeline and collection of codes. This pipeline can generate data products that are fully compatible with the FLUXNET2015 dataset. Its first version was made available publicly in September 2018, and has been updated with improvements and fixes since then. ONEFlux is now being integrated into the AmeriFlux data pipeline. This addition is made possible by the improvements to the products mentioned before. In particular, ONEFlux executions take full advantage of the new AmeriFlux quality control protocols, allowing more robust execution of the codes in ONEFlux. The products in this pipeline include gap-filling of micrometeorological, flux, and other environmental variables, partitioning of CO₂ fluxes into respiration and photosynthesis, estimation of uncertainty from both the measurements and data processing steps, among others. Besides the integration into the AmeriFlux pipeline and creation of a new AmeriFlux data product, we are now working on the next steps for the ONEFlux pipeline. Examples of ongoing work include adapting modules for using more recent reanalysis datasets to create downscaled products for micrometeorological data and fill long gaps in these types of variables; updating key steps in the pipeline with recent developments in the community, e.g., to use different light response functions for CO₂ flux partitioning and handling long time-series more consistently across steps. This poster will show the current state of the ONEFlux pipeline, its integration into the overall AmeriFlux pipeline and new data products for AmeriFlux sites, and future development plans.

Poster #9-42**Simple Footprint Approximation for Better Interpretation of the Spatiotemporally Dynamic Eddy Covariance Flux Data**

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Project: AmeriFlux Management Project

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

Global and regional networks of eddy covariance towers such as AmeriFlux and FLUXNET provide the largest synthesized data sets of CO₂, H₂O, energy, and other GHGs fluxes. This includes the FLUXNET2015 and AmeriFlux BASE data sets that have been widely used in many studies to parameterize, calibrate, and validate models such as those from satellite-based remote sensing and land-atmosphere climate models. While the eddy covariance data are well recognized for their rich temporal information, their spatially dynamic nature as a result of the varying source areas from time to time (i.e., so-called flux footprint) is often overlooked. Up to date, the network-wise tower footprint information is still unavailable and that leads to uncertainties and potential biases when comparing the flux data with model results often designated at fixed grids/pixels. This study aims to evaluate the footprint representativeness of the AmeriFlux sites and test the potentials of simple footprint approximation for better interpretation of the spatiotemporally dynamic flux data. We calculated the footprint climatology for ~50 AmeriFlux sites that provided all variables required for two-dimensional analytical footprint models (e.g., cross-wind variance, friction velocity, Obukhov length). We then evaluated the potential bias of source areas by comparing the spatially-explicit flux data against results from several remote-sensing vegetation indices and model results. Our preliminary results showed that the footprint information largely improve the model-data comparability, especially at sites that have relatively limited fetch and/or are located within a relatively heterogeneous landscape. Last, we demonstrated a few alternative approaches for calculating footprints when cross-wind variance, one of the required but usually unavailable key variables, was not provided. Despite the alternatives may not provide spatially-explicit footprints as accurate as the commonly used two-dimensional analytical footprint models, we showed their application values for improving the interpretation of the spatiotemporally dynamic flux data, especially for those earlier data or inactive sites where it is infeasible to recalculate the flux data to include the currently missing cross-wind variance.

Subsurface Biogeochemical Research

**Argonne National Laboratory
SBR Science Focus Area**

Poster #22-25**Argonne Wetland Hydrobiogeochemistry SFA**

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

Within wetlands, movement of water and biogeochemically catalyzed transformations of its constituents determine the mobility of nutrients and contaminants, the 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 studies wetland hydrobiogeochemistry with a focus on a riparian wetland field site within Tims Branch at the Savannah River Site. This site is representative of many riparian wetlands found in humid regions of the Southeast that have C-rich soils and high Fe content. However, it is unique in that it received large amounts of contaminant metals and uranium as a result of previous industrial- scale manufacturing of nuclear fuel and target assemblies. Understanding the function of the wetlands in relation to control of water quality, including the concentration of metals and uranium within the soluble and particulate components of groundwater and surface waters of Tims Branch addresses the goal of the SBR Program to *advance a robust, predictive understanding of watershed function*.

The overarching hypothesis of our work 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 determine water quality: *sediment, rhizosphere, and stream*. These three focus areas are interdependent and are considered as a whole for a systems-level understanding of our overarching hypothesis. 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 molecular-scale biogeochemical processes that affect Fe, C, and contaminant speciation within the wetland sediment, rhizosphere, and stream environments; and*
2. *In-depth understanding of hydrologically driven biogeochemical controls on the mass transfer of Fe, C, and contaminants within wetland sediment, rhizosphere, and stream environments.*

Holistically addressing hypotheses related to these two knowledge gaps organizes the SFA in its development of a hydrobiogeochemical conceptual model of the Tims Branch riparian wetland.

Poster #22-26**Iron Flocs as Biogeochemically Dynamic Reservoirs of Uranium in Tims Branch Wetlands, Savannah River Site**Edward O'Loughlin,^{1*} Maxim Boyanov,^{1,2} Daniel Kaplan,³ Kent Orlandini,¹ Pamela Weisenhorn,¹ and Kenneth Kemner¹¹ Argonne National Laboratory, Argonne, IL;² Bulgarian Academy of Sciences, Sofia, Bulgaria;³ Savannah River National Laboratory, Aiken, SC;**Contact:** oloughlin@anl.gov

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>

The Argonne *Wetland Hydrobiogeochemistry* SFA studies wetland hydrobiogeochemistry centered on a riparian wetland field site within Tims Branch at the Savannah River Site. Research is focused on hydrologically driven biogeochemical processes within three critical zones: *sediment*, *rhizosphere*, and *stream*. The dynamic nature of the processes occurring within the stream zone is illustrated by the presence of flocs, which are multicomponent assemblages of microbes, minerals, and non-living organic matter that are often found in freshwater ecosystems, including wetlands. Abundant orange and reddish-brown flocs have been repeatedly observed at multiple locations along Tims Branch. Analysis of these flocs by ICP-OES and XAFS spectroscopy revealed that the flocs contained high levels of Fe (9.7%)—in the form of ferrihydrite (83%) and lepidocrocite (17%) as determined by Fe K-edge EXAFS spectroscopy—P (2.7%), S (1.2%), and Al (0.4%) on a dry mass basis. The flocs contained 320 ppm U and preliminary U L_{III}-edge EXAFS analysis indicates that it is U(VI) in the form of a U oxyhydroxides phase. The concentration of U in floc material was 5.5 times greater than the highest concentration of acid-extractable U in streambank sediments collected at the same time as the floc, indicating the potential importance of flocs in controlling U transport at the site. The stability of flocs varies over time and is dependent on a multitude of physical, chemical, and microbiological processes within the floc and the surrounding water; however, the specific factors controlling the frequency and locations of floc formation and dispersion in Tims Branch are unknown and the focus of current studies. In addition, flocs 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 likewise 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. The results of our initial studies of Tims Branch flocs suggests that they represent a significant, previously unidentified reservoir of potentially mobile U, and as such are the focus of further investigation. Given that iron flocs are frequently observed in a broad range of wetland environments, our studies of iron floc formation in Tims Branch and their impact on U speciation and transport expands our understanding of their role in the speciation and cycling of trace elements in wetlands.

Poster #22-28**Modeling Microbial Controls on Biogeochemical Processes at the Savannah River Site**

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

The Argonne Wetland Hydrobiogeochemistry SFA studies wetland hydrobiogeochemistry centered on a riparian wetland field site within Tims Branch at the Savannah River Site, focusing on hydrologically driven biogeochemical processes within three critical zones: sediment, rhizosphere, and stream. Microorganisms play a fundamental role as mediators of the biogeochemical processes happening in and across these compartments and their activity can result in the sequestration or release of contaminants such as U, as well as the movement of C through the ecosystem. Early 16S amplicon characterization of the microbial community shows that organisms within the *Proteobacteria*, *Nitrospirae*, and *Chloroflexi* phyla are abundant within the sediment compartment at this site, while highly abundant members of the flocc communities within the stream compartment include *Sideroxydans*, members of the *Methylococcaceae*, *Thiovirga*, *Desulfuromonadales*, and many *Betaproteobacteria*. These data were processed in KBase through a newly co-developed pipeline enabling the processing of amplicon data and the generation of microbe-microbe and microbe-metabolite interaction networks to identify common/widespread interactions, stable interactions, critical interactions, and putative keystone species from these samples. This utility of this approach is demonstrated with data collected from the Argonne Wetlands sites. Implications for the incorporation of microbial metabolic activity into reactive transport models will be discussed.

Poster #22-27

Savannah River Site Sediments: Biogeochemistry and U speciation

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

The Argonne SBR SFA is focused on hydrobiogeochemical investigations of a wetland field site (Tims Branch at the Savannah River Site), which is representative of many riparian environments and unique in that it received large amounts of contaminant metals (Ni, Cr, Cu, Pb) and uranium (U) during the manufacture of fuel and target assemblies. The radiological contamination along Tims Branch was mapped using aerial and field-deployable detectors, and sediment cores were collected at locations with elevated U concentrations.

Sediment profiles consisted of organic-rich layers (OL) overlaying mineral layers (ML). Acid digestions indicated elemental content ranging from constituents of the native minerals (e.g., Mg, Al, K, Ca, and Ti) to legacy contaminants (e.g., Cr, Ni, Cu, Pb, and U). The OL was enriched in U (44.5 ± 17.1 ppm) relative to the ML (6.38 ± 2.19 ppm). Microbial community analysis (16S rRNA) showed a diverse microbial population, dominated by sequences from the phyla *Proteobacteria*, *Nitrospirae*, *Chloroflexi*, and others. Fe K-edge XANES indicated 13% Fe(II) in the unsaturated portion of the OL and 30% and 26% in the saturated portions of the OL and ML, indicating the presence of reducing conditions. U L_{III}-edge XAFS spectroscopy indicated that in the unsaturated portion of the OL and in the ML, U was present as U(VI), whereas in the saturated portion of the OL >95% of the U was present as mononuclear U(IV) that rapidly oxidized when exposed to air. Oxic/anoxic incubations of the sediments with glucose indicated a facile and reversible transition between adsorbed U(VI) and mononuclear U(IV) species.

Previous studies at Tims Branch concluded that U(VI) is the predominant species; our new observations of variable U oxidation state with depth and location of the core—as well as the stabilization of mononuclear U(IV) species in the organic-rich layer—suggest that there are significant knowledge gaps in our understanding of the processes responsible for the mobilization of U. We also carried out experiments to understand the role of organic matter in the U(IV) species formed at the field site. Building on prior SFA work, we reduced TiO₂-adsorbed U(VI) in the presence of humic acid (HA). The U(IV) speciation was determined by EXAFS spectroscopy, which suggested U(IV) complexation with the HA. Similarly, the siderophore DFOB was found to complex U(IV) following reduction of a U(VI)-DFOB complex adsorbed to NAu-2 clay. The mechanistic understanding provided by these results improve our ability to predict U transport using Reactive Transport Models.

Subsurface Biogeochemical Research

**Lawrence Berkeley National Laboratory
SBR Science Focus Area**

Poster #21-35**Watershed Function SFA: Hydrological and Biogeochemical Dynamics from Genomes to Watershed Scales**

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Climate change, extreme weather, fires, land-use change, and other disturbances are significantly reshaping interactions within watersheds throughout the world. While mountainous watersheds are recognized as the “water towers” for the world, hydrological processes in watersheds also mediate biogeochemical processes that support all terrestrial life. Developing a predictive understanding of how watersheds respond to disturbances is challenging, as complex, multi-scale interactions can lead to a cascade of effects on downstream water availability and quality. Although these interactions can have significant implications for energy production, water availability, water quality, agriculture and other benefits valued by society, uncertainty associated with predicting watershed hydrobiogeochemical behavior remains high.

The Watershed Function Scientific Focus Area (SFA) is reducing this uncertainty through development of a predictive understanding of how mountainous watersheds retain and release water, nutrients, carbon, and metals. In particular, the project is investigating the impacts of early snowmelt, drought, and other disturbances on watershed hydrobiogeochemical dynamics over seasonal to decadal timescales. While the development of novel watershed conceptualizations and approaches are expected to be broadly transferable, our current research is undertaken within a headwater catchment of the Upper Colorado River Basin – the East River watershed. This watershed has evolved into a so-called “Community Watershed” – a platform for advancing indivisible watershed problems through nucleating and connecting National Lab and University- based research. Characterized by sharp gradients in elevation, climate, vegetation, biogeochemistry and hydrogeology, a system-of-systems approach is being used to predict the integrated watershed response to disturbance. This approach involves intensive investigations in a limited number of archetypal subsystems and scale-adaptive approaches to simulate the aggregated response of the subsystems. Given extreme weather contrasts in recent years, the watershed has served as an ideal ‘natural laboratory’ for investigating the impact of annual variations in snow pack thickness and melt timing on subsystem and aggregated watershed hydrobiogeochemistry, including nitrogen exports.

Recent Watershed Function SFA research has led to numerous insights and capabilities including: acquisition and use of extraordinary watershed data layers to characterize the organization of the watershed; quantification that early snowmelt significantly influences bedrock-through-canopy interactions, including rapid infiltration, groundwater recharge and baseflow – and that the subsurface hydrobiogeochemical activation region varies with snow accumulation; discovery of how the below-snow microbial community influences nitrogen exports; use of snowmelt experiments to discover that earlier snowmelt leads to great synchrony in greening and flowering across elevation gradients; a predictive understanding of how river stage, microbial community and meander permeability influences riparian zone nitrogen exports; and the development of new scale-adaptive modeling and data management capabilities. This poster will describe the Watershed Function SFA scientific goals, approaches, key study sites, and collaborators, and will also summarize select recent achievements.

Poster #21-36**Hillslope Responses to Snowmelt: Approaches for Constraining Predictions of Subsurface Flow and Transport Distributions, and their Downgradient Contributions to Surface Waters**

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Major segments of hydrologic and elemental cycles reside underground, where their complex dynamics and linkages to surface waters are obscure. Field measurements are being used to develop conceptual, algebraic, and numerical models for delineated seasonal dynamics of subsurface flow and transport along a lower montane hillslope in the Rocky Mountains (Colorado, USA), where precipitation occurs primarily as winter snow and secondarily as summer rainfall, and discharges into the East River, a tributary of the Gunnison River. Hydraulic and geochemical measurements down to 10 m below ground surface supported application of transmissivity feedback to describing subsurface flow and transport through three zones: soil, weathering shale, and saturated fractured shale. From water mass balance, groundwater flow was predicted to depths of at least 85 m. Snowmelt during the high snowpack water year (WY) ²017 sustained flow along the weathering zone and downslope within the soil, while negligible shallow downslope flow occurred during the low snowpack WY²018. We introduce subsurface concentration-discharge (C-Q) relations as a framework for explaining hillslope contributions to C-Q patterns observed in rivers, and demonstrate their calculations based on transmissivity- predicted flow rates and measured pore water specific conductance (SC) and dissolved organic carbon (DOC) concentrations. Comparisons with SC in the East River show that major ions in the hillslope pore waters, primarily from the weathering and fractured shale, are about 6 times more concentrated than in the river, indicating solute loads are disproportionately high, even while flow from this site and similar regions are small. The methodology developed here can be applied to transect in different representative environments within watersheds in order to link their subsurface exports to river C-Q responses. A ²-D reactive transport model that can resolve lateral fluxes through the unsaturated and saturated zones of the lower montane hillslope has been developed using TOUGHREACT. Simulation results show distinct spatial and temporal signatures in hydrologic budgeting across the transect. In particular, greater evapotranspiration rates and higher soil water storage are obtained in the floodplain as compared to upslope regions. Moreover, upslope regions show more sensitivity to seasonal variations and changes in snowmelt timing than the floodplain. Future modeling efforts will focus on quantifying the role of changing winter precipitation regimes on hillslope and riparian contributions to dissolved carbon and nitrogen exports to the river.

Snowpack Dynamics and Coupled Plant-Soil-Microbial Processes in a Mountainous Watershed

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In mountainous systems with seasonal snow-cover, interactions between vegetation, microorganisms and regolith properties are key to the retention or loss of water, nutrients and other elements. Snowpack dynamics, including snow depth and timing of snowmelt, shape these interactions. Vegetation phenology, regulated by environmental cues such as photoperiod, soil and air temperature, is tightly coupled to snowmelt date. The timing of snowmelt is changing, occurring earlier, shifting vegetation phenology with consequent impacts on the hydrology and biogeochemistry of mountainous watersheds. As part of the Watershed Function SFA at East River, CO, our goal is to build a mechanistic understanding of how coupled plant-soil-microbial processes respond to perturbations such as early snowmelt and project changes in exports from watershed subsystems to the river.

Over the last three years we have observed record high and low snowpacks and have manipulated snowmelt date at select locations. Early snowmelt (natural or manipulated) advances vegetation greening, shifting peak evapotranspiration (ET) earlier which in some watershed subsystems results in an ET-induced foresummer drought and compressed growing seasons. Across the watershed elevation gradient, greater synchrony in greening and flowering was observed in low snow years and early snowmelt, shifting typical ET distributions with implications for water and nutrient exports.

River nitrogen discharge peaks during snowmelt and isotopic studies have demonstrated that river nitrate is primarily derived from nitrification of terrestrial ammonia rather than atmospheric deposition. Under the insulation of a deeper snowpack, microbial activity is at its highest and microbial biomass blooms, retaining N until snowmelt when a crash in biomass is observed. Using metagenomic, transcriptomic and metabolic approaches we have documented the importance of volatile organic compounds that support microbial growth, increases in phage abundance associated with the microbial biomass crash, and significant archaeal nitrification associated with the observed nitrate pulse at snowmelt. These processes are muted under low snowpack conditions demonstrating that snowpack dynamics effect both vegetation and microbial phenology and the timing of nutrient availability.

To scale beyond intensively studied locations, we have developed simultaneous above and belowground sensing platforms to relate surface observables to subsurface physical, chemical and biological properties. A strong relationship between canopy phenology and subsurface electrical conductivity (EC, a proxy for soil physical properties and water availability) was observed and related to hillslope factors that are also strong predictors of vegetation distributions. Efforts to evaluate such surface-subsurface covariance are ongoing at the watershed scale using LiDAR and hyperspectral data.

Poster #21-38

Subsurface Rock Records and Water Signatures of Metal and Nutrient Mobilization from Mancos Shale at East River

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It is increasingly appreciated that the biogeochemical weathering of rocks and minerals in the zone between topsoil and competent bedrock can provide an important source of nutrients and metals into groundwater. Studies at the East River watershed, and across the Upper Colorado Basin, have linked Mancos shale weathering to seasonal inputs of salinity, nutrients and metals including contaminants into floodplains and rivers. Knowledge is lacking, however, of the primary controls on the rates of shale weathering and the impacts of weathering products on biogeochemical cycles and river quality. In 2017 and 2018, complementary field and laboratory studies addressed the pathways and consequences of shale weathering at and around the PLM intensively monitored hillslope transect at East River. First, elemental, chemical and mineral analysis of drill cores, soil-to-bedrock pits and weathering fracture surfaces revealed shale weathering profiles at the 10-m and 10-mm length scales. Second, time series of vertically- resolved groundwater chemistry at instrumented wells, provided time-series data on the concentrations of inorganic and inorganic solutes derived from shale weathering. Third, batch and column incubations of unweathered shale isolated key geochemical and microbial processes that liberate and cycle metals and nutrients. The groundwater data show Mancos Shale to be an important source of nitrogen, sulfur, phosphorous, and metals that are preferentially mobilized in an actively weathering zone between base-flow water table and top soil. The laboratory studies establish the role of clay minerals in the release of ammonium and *in situ* microorganisms for rapid nitrification. Element and mineral patterns in the rock record show evidence for both export and accumulation of reactive minerals and metals with a strong dependence on groundwater and pore water pH and redox state. A shale weathering model is under development in CrunchFlow that will enable the prediction of nutrient and metal mobilization, retardation and export in response to changing hydrologic patterns.

Poster #21-39

Phenological Responses to Earlier Snowmelt and Potential Impacts on Evapotranspiration in a Colorado River Headwater Basin

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Plant emergence, growth, and flowering phenology in mountain meadows are driven by either snowmelt timing (i.e. sites reach 0% snow water equivalents, SWE), temperature, photoperiod, or combinations of these. In mountain watersheds, meadows cover vast areas, especially at higher elevations. The East River, a headwater basin of the Colorado River, is experiencing increased spring air temperatures (mean daily +1.4°C/decade at SNOTEL #380, 1987-2018) and a greater frequency of dust deposition on the snowpack. Snowpack is also decreasing across Colorado and many mountain regions of the Western US. As a result, snowmelt is earlier with consequences for plant phenology that may alter water fluxes and element retention. We expect that early snowmelt in combination with warmer spring temperatures will lead to earlier greening at all elevations with a greater shift for higher than lower elevation regions of the mountain watershed. We have developed an approach to relate phenology to soil water content to determine potential impacts of early plant growth on evapotranspiration.

Climate years 2017 and 2018 were warm years in the mountains of Colorado. Air temperatures were greater than historical mean temperature and on some days exceeded historical maximum temperatures. Snowmelt was earlier in 2018 compared to 2017 due to substantially less snow. Across an elevation gradient (2774-3597 m) within the watershed, we observed snowfree conditions 21-49 days earlier due to this interannual variation, and in 2018 further advanced snowmelt by 10 days experimentally. In warm years, earlier snowmelt leads to earlier greening and increasing synchronization of plant growth and flowering across elevation from montane to alpine life zones. The advance in greening was far greater for the upper elevation sites 3475 m and higher, resulting in greater synchronization than expected based on years of working in mountain systems. When the window of time over which elevations reach 0% SWE shrinks, water inputs to soil, plants and rivers do not extend over time. Asynchronous snowmelt is critical to sustain water inputs prior to when seasonal rains begin (typically mid-July). Among the more than 40 species monitored, we observed earlier plant senescence and plants that remained green but for which production was low. A cold year or a cold spring would greatly benefit our understanding of plant phenology and its effect on water supply, yet, the likelihood of this is extremely low.

Poster #21-40

River Corridor Processes Impacting Nutrient and Metal Export in the East River

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Project: Berkeley Lab Watershed Function SFA

Project Website: watershed.lbl.gov

The river corridor is generally defined as including the main river channel as well as the following associated River Corridor Elements (RCE): hyporheic zones, meanders, lagoons, sediment deposits, riparian zones, floodplains, topographic hollows, beaver dams, off-channel wetlands, and other key landscape features. These features are increasingly recognized as important components of headwater catchments. Hydrologic connectivity along river corridors and across RCE is considered to be one of the key controls of geochemical exports of metals and nutrients to streams but this connectivity changes with climatic and seasonal conditions, e.g. spring snowmelt or monsoon storms, making the emergent functioning of the system dynamic across time and space. The efforts reported here have focused on quantifying and modeling the biogeochemical processes and hydrologic connectivity taking place in particular RCE to assess and simulate their impact on geochemical export in the East River. The RCEs focused on to date include vertical and horizontal hyporheic exchange across meanders and river bedforms supported by laboratory experiments, modeling simulations, and extensive field geochemical sampling. Our extensive research activities have revealed some novel insights including: 1) meander geomorphology supports extensive lateral redox gradients which is shown to enhance metal export from the meander to the river; 2) sediment heterogeneity is the determining factor for whether a meander is functionally classified as 'oxidizing' or 'reducing'; 3) hydrology perturbations combined with knowledge of vertical hydro-stratigraphy together enhance later redox zonation and Fe, C export, and 4) evidence of substantial vertical redox zonation and anoxic microzone development beneath the riverbed that may support substantial and enhance river denitrification as climate warms. Our future river corridor efforts will focus on vertical hyporheic exchange with a particular emphasis on the development of a mechanistic stream/benthic/hyporheic system model with various hypothesis testing capabilities for understanding the role and implications for decadal scale nitrogen exports. In addition, the preliminary work has indicated the potential importance of off channel wetlands as important RCEs whose functioning and impact require further development. Lastly, it is a key goal of this effort to develop numerical scaling schemes based on the interconnection of RCEs that can be applied across large sections of the East River as well as other adjacent drainages.

Poster #21-46

Factors Governing Microbially-Mediated Geochemical Processes and Microbial Community Composition Across Watershed Ecosystem Compartments

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Microorganisms mediate virtually all geochemical cycles in the terrestrial near-surface. While the predominant transformations that community members can perform are expected to vary considerably with site-specific conditions, we do not know which factors are most important or how functions are distributed across landscapes. We are investigating the drivers for release and uptake of nutrients and other compound transformations across a watershed by subdividing the system into major compartments, three of which are being intensively studied. First, we identified four major vegetation types and are evaluating their distinct soil ecosystems in the upper reaches, mid watershed and lower reaches of the East River, Colorado. Results show significant variation in both microbial community composition and metabolic potential as a function of vegetation types and soil depths. Location in terms of watershed longitudinal position also exerts a significant impact on metabolic potential of microbial communities. We find that vegetation type and location are important determinants of nitrification and C1 metabolism while soil depth influences processes such as organohalide reduction, impacting fluxes of compounds across hillslopes, into riparian zone soils, and exports to the river. Second, we considered position on the hillslope as a control on microbial community structure and functions within the watershed. By analysis of soil and sub-soil communities, we show substantial variation with depth as well as some lateral variations, particularly associated with proximity to the East River. We found that the intersection of the hillslope and riparian zone at the floodplain is compositionally and functionally distinct from communities on the hillslope. Microbial communities in the floodplain soils are similar to those found throughout the soils of the riparian zone. Third, we intensively sampled three meander floodplains along the East River corridor to test for variation within the regions circled by the river and to compare them to each other. Gradients in community composition and metabolic potential occur within the soils flanking each meander. However, there are striking features shared by the meanders. Notably, certain strains of bacteria are consistently abundant across floodplains and play similar roles in biogeochemical cycling at each site. For instance, the capacity for sulfur metabolism seems persistent among organisms that are abundant across sites. Overall, the results have begun to elucidate which parameters are more and less important for shaping community composition and microbial capacities within the watershed. Additionally, this inventory of watershed microbial metabolic potential is being used to inform reaction networks in models across scales.

Spatial and Temporal Dynamics of Nitrogen within a Mountainous Watershed

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A widely held conceptual model of pristine mountainous watersheds maintains that ecosystem productivity is limited by nitrogen availability. Work within the current phase of the SFA supports and contradicts this paradigm, indicative of a temporally heterogeneous ecosystem. For example, our recent efforts have demonstrated that hydrological export of dissolved inorganic and organic nitrogen during the most intense periods of nitrogen demand (i.e., the growing season) can be high (indicative of no limitation), and extremely low (indicative of nitrogen limitation). Given the importance of headwater streams for downstream nitrogen dynamics, a more nuanced characterization and quantification of the main sources and sinks for nitrogen within the watershed can improve understanding of the fate of nitrogen.

Efforts within the first phase of this SFA have focused on identifying the ecosystem traits (e.g., geology, geomorphology, vegetation, microbial activity) controlling the fate of nitrogen. First phase studies have shown that shale bedrock (~ 4.2 kg ha yr⁻¹ and 3.3 kg ha yr⁻¹ in 2017 and 2018), alongside atmospheric deposition (~ 2 kg ha yr⁻¹), is a significant source of both NH⁴⁺ (through weathering and cation exchange), and NO³⁻, via *in situ* nitrification, at the East river. This input can be several-fold larger than the hydrological export of NO³⁻ from the East River watershed, indicating significant retention and storage of nitrogen within watershed vegetation, soils, or aquifer. Indeed, a coarse scale model (HAN-SoMo) informed by PARFLOW, emphasizes the importance of plant processes as critical controls on the retention and release of nitrogen, and denitrification as a critical watershed loss term for nitrogen, up to four times larger than hydrological export. The timing of snowpack formation, the depth of that snowpack, and snowmelt are important factors in determining this retention and release of nitrogen. First phase observations demonstrate that a deep snowpack thermally insulates the soil, maintaining soil temperatures above freezing and facilitating soil microbial growth and activity. The subsequent snowmelt period can induce a crash in microbial biomass and a significant pulse of nitrogen release. However, a late accumulating and shallow snowpack, with a persistent layer of frozen soil (during the winter of 2017-2018), showed no overwinter immobilization of nitrogen in microbial biomass and no appreciable release of nitrogen. Understanding gleaned from measurements and modeling efforts performed in the first phase of this program will contribute towards our second phase goal of using historical nitrogen records to better predict the future watershed nitrogen cycle.

Poster #21-44

Snow and Landscape Controls on Recharge and Groundwater Flux to Streams

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Understanding mountain hydrology is complicated by the tight coupling of snow processes, vegetation and topography, while the importance of groundwater in these systems and its sensitivity to climate remain uncertain. In this framework, spring snowmelt is one of the major sources of recharge. To address challenges, we combine snow observations across spatial and temporal scales, groundwater gas tracers, and an integrated hydrologic model of the East River, CO to explore stream water source, depth of hydrologically active groundwater, and first-order controls on recharge as well as baseflow age distributions. Use of Lidar-derived snow water equivalent allows us to implicitly account for nuances in storm patterns, snow redistribution processes related to wind and avalanche, and capture high elevation snowpack accumulation and persistence important for water resources. Results indicate 35% of streamflow comes from groundwater to independently validate Carroll et al. (2018) assessment using end-member mixing analysis. We find groundwater flow to streams remains stable across the multi-decadal simulation (water years 1987-2018) despite variability in snow accumulation and melt. While there is stability in simulated groundwater flow volumes, the relative contribution of groundwater to streams varies considerably (21-52%) as a function of aridity and the tight coupling between basin-scale ET and interflow. During low snowpack years, ET/P increases at the expense of lateral flow through the soil zone. Resilience of groundwater volumetric flux is dictated by changes in groundwater storage. The responsiveness of groundwater storage to snow accumulation occurs because the majority (~53%) of groundwater moves through the permeable alluvium and shallow fractured bedrock that are relatively well connected to surface water input from snowmelt. The remaining groundwater component, however, moves through deeper fractured bedrock and steeply dipping sedimentary strata, with drier scenarios lowering water table depths and extending circulation downward. Our results support the hypothesis presented by (Carroll et al., 2018) that the upper subalpine focuses groundwater recharge in mountain systems. However, we find that while coupled seasonal vegetation and snow dynamics are particularly important in the lower reaches of the basin, the dominant control on maximum recharge in/above the upper subalpine is topographical. Lastly, baseflow ages derived from gas tracers (SF₆, CFCs) and numerically generated particle tracking independently agree that median age of groundwater discharging to streams is approximately 10 years with numeric modelling highlighting the importance of geologic structure driving deeper flow paths and older travel times. We conclude that deeper groundwater is an important component of mountain hydrology and should be explicitly included in water budgets for improved predictive capability.

Reference:

Carroll, R. W. H., Bearup, L. A., Brown, W., Dong, W., Bill, M., & Williams, K. H. (2018). Factors controlling seasonal groundwater and solute flux from snow-dominated basins. *Hydrological Processes*, 32(14), 2187–2202.

<http://doi.org/10.1002/hyp.13151>

Poster #21-43

Energy Balance Dynamics, Plant Water Use, and Subsurface Residence Times in the East River, Colorado

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Understanding the integrated water budget of mountainous watersheds requires knowledge of not only the distribution and partitioning of groundwater, surface water, and water used by vegetation, but also the inextricable link between energy fluxes with the atmosphere at the land surface. Given that evapotranspiration (ET) is the largest terrestrial water flux and transpiration often comprises 60% of ET, plant water use becomes a primary driver of these fluxes, moderating water availability for downstream use. A combination of models and observations are used here to understand the transient movement of water and energy across the earth's critical zone within the East River, Colorado. With the use of high performance computing, integrated hydrologic models enable a physically based representation of watershed hydrodynamics in high resolutions. Multi-year simulations of watershed behavior over the last decade at both local (i.e. hill slope transect) and regional (i.e. watershed) scales are performed with the integrated hydrologic model ParFlow-CLM. Results show the transient behavior of above and below ground storage vary drastically with water year, and can be directly used to inform the cascading bio-reactor model, HAN-SoMo, which shows excellent agreement in nitrogen cycling in the East River informed by residence times from the ParFlow-CLM simulations. Additionally, a new Lagrangian particle tracking technique is used to determine the transient movement of water, explicitly representing water source, age, and the associated flow pathways. Simulated fractionation of water with particles is quantified and directly compared to stream flow and depth-refined groundwater well samples. This new approach also enables novel comparisons of the degrees of water fractionation of evapotranspired water, enabling an improved knowledge of under what conditions vegetation water demands are met. Results show that ET residence times are very dynamic, demonstrating strong spatial patterns related to topography, land cover, and properties of the subsurface medium. Finally, the analysis of Eddy Covariance flux tower data shows excellent energy closure during the summer, but difficulties in the winter energy balance. Preliminary work shows that winter energy balance uncertainties are attributed to complex terrain and snowpack dynamics. Future work includes direct comparisons of model energy flux simulations with various land surface models (e.g. CLM and NOAH) and flux tower observation comparisons to determine energy loss seepage terms during the winter season, in addition to future instrumentation in various locations within the watershed.

Poster #21-42

4D Digital Watershed: Advanced Bedrock-to-Canopy Characterization across Watersheds

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Characterizing ecohydrological-biogeochemical processes over heterogeneous watersheds are critical for estimating and predicting integrated hydrological and biogeochemical responses – such as carbon and nutrient exports, water resources and quality – under climate changes and other perturbations. In the Watershed Function SFA, we develop novel watershed- characterization methodology to quantify complex watershed systems across scales, using advanced sensing, inversion, and machine learning approaches. Through explicitly bridging information derived from “on the ground” observations made at the East River Watershed and remote sensing data, we quantify fundamental scientific linkages among interacting processes in the watershed. We integrate multi-scale multi-type datasets, including hydrobiogeochemical point measurements as well as surface geophysics, airborne data and satellite/UAV images. Over the last few years, we have acquired an extensive suite of high-resolution airborne remote sensing data over the watershed, including LiDAR for ground and top-of-canopy elevations, time-lapse NASA Airborne Snow Observatory (ASO) for snow and SWE distributions, NEON hyperspectral mapping for leaf chemistry and plant physiology, and airborne electromagnetic (EM) survey for subsurface structure (jointly with USGS).

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

- Watershed-scale estimation of the shale bedrock porosity and fracture density, obtained through combining airborne electromagnetic data with borehole and surface-based geophysical data.
- Meter-scale mapping of meadow plant communities through the LiDAR/multispectral data fusion, and understanding of their spatial organization depending on soil/topographic characteristics
- Key drivers that regulate watershed vegetation sensitivity to droughts through historical Landsat datasets and random forest machine learning method
- The first watershed zonation map using hierarchical cluster analysis and spatial data layers, which delineates regions that have unique distributions of above-and-below ground properties that are likely to influence subsystem behavior, and thus aggregated watershed behavior
- A novel autonomous above-and-below ground coincident sensing system, tested at the East River Watershed hillslope intensive site to quantify how the relationships between soil moisture and vegetation density evolve during the growing season

By characterizing spatiotemporal (i.e., four-dimensional) variability of critical properties over the watershed, we aim to develop the new 4D Digital Watershed concept for model parameterization and validation of hydrological and biogeochemical simulations. In addition, we plan to use both model and data-driven approaches to co-design our characterization and monitoring network.

Poster #21-41

Geophysical Characterization of Bedrock Properties of the East River Watershed: From Subsystem to Watershed Scale

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A critical aspect to improving our predictive understanding of watershed hydrobiogeochemical dynamics is quantifying the influence of bedrock properties on subsurface flow and transport over a range of space and time scales. To obtain a watershed-scale understanding of the subsurface physical properties of the watershed, we link data of several scales by jointly interpreting geological, remote sensing, airborne Electromagnetic (AEM), detailed geophysical, and wellbore data. Subsystems of subalpine to montane environments were characterized using electrical resistivity tomography (ERT) and seismic refraction tomography (SRT). All of these sites were located within the Mancos shale unit. While subalpine environments generally show high electrical resistivities and high seismic wave velocities, indicative of competent bedrock, the sampled lower montane environment shows considerably lower values in both resistivity and seismic wave velocity. Borehole coring and logging data acquired at the same locations show a distinct change in bedrock characteristics, with subalpine environments having low bedrock porosity and lower montane environments having considerably higher porosities. From this data, we obtained petrophysical relationships that link electrical resistivity and seismic wave velocities to estimated porosities. These relationships were then applied to the spatially extensive AEM data, which also showed a pronounced change in bedrock porosity from low values in subalpine to high values in montane environments. The observations on the subsystem and watershed scale are in agreement with hydrological monitoring and modelling data, confirming the link between geophysical parameters, ecotypes, and subsurface flow properties. We investigate the relationship between local and regional geophysical data with geomorphological and environmental indices to upscale the insights we gained at the subsystem scale to the watershed scale. Eventually, this will allow us to build a 3D model of the subsurface physical properties of the watershed. Such a comprehensive data set forms the basis for quantifying the distributed bedrock-through-canopy responses of the watershed to perturbations, and how these contribute to a cumulative downgradient discharge-concentration signature.

Poster #21-29

Watershed Function Simulation and Aggregation

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Watershed hydrological processes mediate a wide range of biogeochemical interactions, ranging from vegetation growth to elemental and nutrient cycling to contaminant fate and transport. However, there are huge uncertainties associated with predicting how watersheds will respond to such perturbations (e.g., droughts or floods) at space and time scales relevant to the management of environmental and energy strategies. Complementing modeling activities focused on intensive study sites in other components of the Watershed Function SFA, the Watershed Reactor effort aims to understand and predict the aggregated behavior of the system affected by coupled hydrological, energy, and biogeochemical processes. One important challenge is the resolution of hot spots (spatially focused zones of intense hydrological or biogeochemical activity) and hot moments (transient events with potentially outsized impact on system function). As an example, hydrological flow and biogeochemical processes may generate meter scale gradients in concentration in reactive floodplains, and these may need to be captured in models to accurately represent fluxes. Similarly, hillslope processes may be affected by small scale variations in vegetation and slope and weathering depth, all impacting fluxes to the river system. To address these potentially outsized impacts on river quality, we are developing HPC simulations using the IWaSE (IDEAS Watershed Software Ecosystem) for the Lower Triangle and Copper Creek within the East River watershed. Using the Amanzi-ATS package for flow and transport within IWaSE, we make use of variable resolution unstructured grids that focus resolution in the floodplains and other zones where hydrologic and/or biogeochemical hot spots can develop. In addition, we use high resolution hydrological modeling based on the ParFlow-CLM software to calculate travel time distributions for surface and subsurface water within the East River watershed. These are used by both the Han-SoMo bioreactor model, and to analyze the partitioning of water between the surface and subsurface by comparing simulation results with isotopic measurements of river water at various places within the watershed. In Copper Creek, our focus initially is on capturing stream discharge, with the ultimate objective of using reactive transport capabilities within IWaSE to address the question of how variable depth weathering fronts (i.e., O₂ and CO₂ driven) impact watershed biogeochemical fluxes.

Poster #21-30

Data Management Framework for LBNL's Watershed Function Scientific Focus Area

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The Watershed Function SFA project generates diverse datasets at its field site in East River, Colorado, which include hydrological, geochemical, geophysical, ecological, microbiological, and remote sensing data. The datasets are collected by the LBNL project team and obtained from collaborators or other external sources.

The objective of the SFA's Data Management Framework is to provide infrastructure and services to: (1) manage, archive, and publicly release data collected by the SFA as per the [project's data policy](#); (2) enable the SFA team and the broader community to discover and access relevant datasets; (3) perform Quality Assurance and Quality Control (QA/QC) of priority datasets; and (4) enable efficient data collection, data integration, and product generation.

To meet these objectives, the data team has developed a number of tools for data management and preservation, QA/QC, data discovery, advanced search, and visualization. The SFA's data package system provides for internal data archival and curation of project-generated data. It allows authorized users to upload data files with relevant metadata, and download files shared within the project team. The SFA's datasets are publicly released via the ESS-DIVE archive. Priority datasets are run through automated QA/QC algorithms that are based on the application of statistical methods used to identify and flag bad and anomalous data in collected datasets. The data team is developing a brokering service BASIN-3D that integrates diverse project and external datasets in real-time from distributed databases via web services. BASIN-3D is based on the Open Geospatial Consortium's Observations and Measurements standard and is currently implemented to integrate time-series data. It powers a [web portal](#) that enables users to conduct an intuitive search, interactive visualization, and download of integrated datasets. Additionally, a [public interactive map](#) of the East River has been developed to inform the broader community about the SFA's field infrastructure and research activities. Sites can be filtered by their key measurements and other metadata, leading to detailed site landing pages.

The data team is working in cooperation with the science teams to create crosscutting data products and workflows for hypothesis testing and modeling. Standardized field collection sheets and sample tracking were implemented to coordinate the extensive data and sample collection for the NEON hyperspectral ground campaign. The developed QA/QC'ed meteorological data products are being used by the science teams as model inputs for predictions of the water balance processes, including infiltration, evapotranspiration, groundwater recharge, and river discharge, as well as geochemical modeling.

Regional Airborne Geophysical Data Analysis and New 2018 Ground-Based Geophysical Data Collection in Redwell Basin, Colorado

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Geologic controls on groundwater flow, particularly in tectonically and topographically complex mountainous terrain, can be difficult to quantify without a detailed understanding of the regional subsurface geologic structure. This structure can influence the direction and magnitude of groundwater flow through the mountain block, which in turn impacts groundwater composition and the flux of metals and nutrients to the near-surface ecosystem. In support of several ongoing studies in the upper East River and surrounding watersheds in central Colorado, regional-scale airborne electromagnetic (AEM), magnetic, and radiometric surveys were conducted in late 2017 over an area of nearly 500 square kilometers. These data give a new view of the geologic structure underlying the region that is unprecedented in both resolution and spatial coverage.

Inversions of the AEM data indicate good correlation with known geology and help to extend interpretations of geological model structure in this complex mountain watershed. Resistivity values exhibit a large dynamic range over the entire survey area—spanning more than four orders of magnitude—and suggest that AEM data will be useful in distinguishing important geologic features in the study area. Portions of the dataset exhibit strong airborne induced polarization (AIP) effects, including double sign changes, providing additional geological insights and identifying areas that may contain polarizable materials such as disseminated metals, fine grained lithology, or geochemical alteration. Modelling AIP extracts maximum information from the dataset, simultaneously producing more accurate resistivity models and chargeability models that can lead to better constrained geologic interpretations. Finally, ground-based geophysical data collection in 2018 included several transects of surface nuclear magnetic resonance (sNMR) data acquired in Redwell Basin near boreholes MW1 and MW2.1. New sNMR data collection was done in collaboration with Vista Clara, Inc. as part of a DOE SBIR Phase-II project to develop ‘rapid scanning’ NMR technology. Transects of sNMR data help to characterize lateral trends in shallow water content that will be used to extrapolate water level observations and other geophysical measurements at the borehole locations to a larger portion of the basin. These results will aid in the development of more accurate conceptual and numerical models of Redwell Basin’s groundwater flow system.

Poster #21-28

2018 Geologic, Hydrologic, Borehole Geophysical, and Geochemical Data Collection in Redwell Basin, Colorado: Overview and Preliminary Results

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A second round of drilling, sampling, and geophysical/geological data collection activities were performed during summer 2018 in Redwell Basin, an alpine tributary of the East River, Colorado. Redwell Basin contains sedimentary bedrock with extensive sulfide mineralization that produces both natural and mining-related acid-rock drainage. The central objective of our project is to characterize and quantify controls on the flux of water and metals in the basin's bedrock groundwater flow system. A second deep borehole, MW2.1, was drilled adjacent to Redwell Creek at mid-elevation (3267 m) to complement existing bedrock well MW1 located high in the watershed (3412 m). MW2.1 was drilled to a total depth of 46 m with nearly complete core recovery. High rates of artesian flow were encountered, preventing deeper drilling. Ten-meter interval open-hole packer tests were performed, indicating hydraulic conductivities of 10^{-7} to 10^{-6} m/s, and a multi-level monitoring well with three different screens was installed. A full suite of borehole geophysical logs were recorded using standard tools, plus acoustic and optical televiewer, full wave form sonic, spinner flow meter, and nuclear-magnetic resonance (NMR). A shallow (10 m) borehole was also drilled adjacent to MW1 and completed with six discrete sampling ports for vadose zone soil gas and shallow groundwater sampling.

Three additional shallow piezometers were installed in groundwater discharge zones to augment the existing network. Forty-five water samples were collected from wells, streams, and other sites, and analyzed for major ion and trace element chemistry and stable isotopes of water. A subset was also analyzed for Sr isotopes and age tracers (tritium, sulfur hexafluoride, and noble gas isotopes). Rock samples were collected from the MW2.1 drill core for permeability/porosity, petrophysical, petrographic, X-ray diffraction, and other chemical analyses. Finally, geological data collection included a second round of outcrop mapping of hydrothermal alteration and brittle structures, as well as comprehensive logging of stratigraphy, structures, and mineralogy in the MW2.1 core. Acquisition of analytical results, data interpretation, and merging of 2017 and 2018 data are ongoing, and preliminary results will be presented. One key initial finding based on available hydraulic head, water age, and water chemistry data is an apparent lack of hydraulic connection between the shallow active water-table aquifer and deeper (>30 m), much older groundwater in upper Redwell Basin.

Subsurface Biogeochemical Research

**Lawrence Livermore National Laboratory
SBR Science Focus Area**

Poster #21-47

The LLNL BioGeoChemistry of Actinides SFA

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Project: SFA BioGeoChemistry of Actinides, LLNL

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

The focus of the BioGeoChemistry of Actinides SFA is to identify and quantify the biogeochemical processes and the underlying mechanisms that control actinide mobility in an effort to reliably predict and control the cycling and migration of actinides in the environment. The research approach includes (1) Field Studies that capture actinide behavior on the timescale of decades and (2) Fundamental Laboratory Studies that isolate specific biogeochemical processes observed in the field. Located at Lawrence Livermore National Laboratory, this SFA harnesses the capabilities and staff expertise unique to this national laboratory to advance our understanding of actinide behavior in the environment and serve as an international resource for environmental radiochemistry research. In this SFA, we have selected five field research sites. Four sites were selected because they represent a diverse range of hydrologic and biogeochemical conditions (Ravenglass Estuary, UK; Pond B, Savannah River Site; Z-9 trench, Hanford reservation; E-tunnel ponds, Nevada National Security Site). The sites range from oxic to anoxic, vadose zone to saturated zone, pH 5 to 8, low to extremely high organic matter, low to high actinide concentrations, low to high ionic strength, and all have a well documented long-term contamination history (~60 years). The fifth site (the Radflex facility) is a unique simulated contamination site that is formulated to test the evolution of specific actinide source material over an extended timeframe. We are focusing on three broad categories of actinide stabilization which include co-precipitation of Pu in common minerals, the role of redox cycling on actinide stabilization on mineral surfaces, and the role of microorganisms and their exudates in actinide mobilization and immobilization. The combination of field and laboratory experiments are exploring actinide migration behavior at environmentally relevant timescales (years to decades), identifying the specific processes controlling the long-term behavior of actinides, and establishing conceptual models of actinide evolution under hydrologically diverse conditions.

Poster #21-48

Plutonium Migration Behavior at Hanford – Trench 216-Z-9

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Located on the Columbia River, the Hanford Site (WA) was established in 1943 to produce plutonium (Pu) for the Manhattan Project and actively reprocessed Pu for nuclear weapons from 1944-1989. Over 184 kg of Pu along with other radionuclides were released into the environment during Hanford site operations. As part of the LLNL BioGeoChemistry of Actinides SFA, we are focusing on understanding the processes controlling Pu migration at the disposal site trench 216- Z-9, located at site 200 west. Over 4 million L of Pu-laden reprocessing waste was released directly to the sediments in this trench between 1955 and 1962. The acidic waste stream was rich in organics, high ionic strength and contained a number of different reprocessing related components (*e.g.* actinides, fission products, CCl₄, lard oil *etc.*).

In the Z-9 trench, most of the Pu precipitated immediately within the first decimeters of the trench as PuO₂ and Pu-polymers or -hydroxides. However, a small fraction migrated deep into the subsurface vadose zone to depths of 37 m. A correlation between Pu and organic components was found in some cases, as well as correlation with Fe and P. However, the mechanisms controlling subsurface migration have not been established. The goal of this project is to identify the Pu migration mechanisms and develop predictions for Pu mobility and potential groundwater contamination at environmentally relevant timescales.

Preliminary experiments have shown that the majority of Pu (approx. 99% from a 1×10^{-9} mol/L solution of Pu(IV)) coprecipitates with Al-hydroxides at $\text{pH} \geq 3$ and thus will be immobilized as a function of waste acid neutralization. Ongoing experiments are examining the structural incorporation of Pu into these Al/Fe co-precipitate phases and their stability in terms of Pu retardation, and possible formation of mobile Pu complexes with Al, Fe and/or P.

Furthermore, we are investigating the influence of organic waste components (*e.g.* TBP and its degradation products) on the migration behavior of Pu in the presence of high nitrate solutions in combination with organic solvents (*e.g.* kerosene, dodecane). Pu partitioning behavior is initially being examined in simple batch systems where pH, minerals, organic components, and ionic strength are varied. Knowledge gained from batch experiments will be applied in subsequent more complex column experiments that will mimic environmental conditions using Hanford sediments and an artificial waste solution containing relevant waste components. The goal of this effort is to identify the specific processes controlling the long-term behavior of Pu at the Z-9 trench and establish a conceptual models of actinide contaminant evolution at this site under relevant biogeochemical conditions.

Poster #21-49

Actinide Mobility at the Ravenglass Site: The Role of Iron and Redox Cycling

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The LLNL BioGeoChemistry of Actinides SFA is investigating actinide migration behavior at the Ravenglass saltmarsh, 10 km south of the Sellafield site, U.K. Since 1952, authorized liquid radioactive effluents (e.g. Am, Cs, Np, Pu, and U) have been discharged from Sellafield into the Irish Sea. The released radionuclides have been re-dispersed along the North-East Irish sea coast including the Ravenglass estuary, a low energy intertidal saltmarsh. Despite periodic study over the past several decades, biogeochemical controls on long-term radionuclide distribution and retention at Ravenglass remain uncertain. Recent work indicates redox conditions shift from aerobic at the sediment surface, to Fe(III) reducing within 12 cm at depth. Shifting redox profiles at this site have the potential to impact the long-term stability of redox active actinides (i.e. Pu, Np, U) and influence actinide release rates into the Irish Sea.

At the Ravenglass site, we are determining actinide desorption behavior from sediments under anoxic and oxic conditions. Currently we have completed Ravenglass sediment desorption experiments (30 cm core, 6 layers) in artificial seawater under anoxic conditions. Analyses to determine the actinide content in the desorbed solutions are currently underway. Follow-on desorption experiments under oxic conditions have begun.

A central hypothesis to our research is that Pu can be stabilized by redox and non-redox mineral alteration processes that lead to Pu incorporation into secondary mineral phases. Minerals of interest include Fe(II)/(III) phases which will likely be subject to dissolution and recrystallization in this dynamic biogeochemical setting. We have monitored the fate of Pu(IV) during the alteration of Pu-doped ferrihydrite to goethite (FeOOH) and hematite (Fe₂O₃). Upon transformation, goethite showed a higher extent of Pu-incorporation than hematite. We have also started similar experiments with magnetite Fe(II/III)₃O₄. Upon synthesis, 98% of Pu remains associated with the magnetite phase. We are currently monitoring the affinity of Pu to the magnetite phase over time and Pu desorption during surface oxidation.

Finally, we are investigating the role of reduced and oxidized forms of humic acid (HA) on Pu sorption/desorption to goethite. In batch systems, both forms of HA demonstrate a similar apparent effect on Pu adsorption. The aggregation of Pu-goethite-HA ternary complexes may enhance the stability of Pu in sediments. However, the redox transformation of both the goethite surface and Pu sorbent in the presence of HA remains unknown. Ongoing research is attempting to disentangle the effect of redox transformations of Pu and iron oxide surfaces in the presence of reduced organic matter.

Poster #21-50

The Influence of Microbial Exudates on Actinide Fate and Transport: Pond B, Savannah River Site

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To examine the role of microbial exudates in the biogeochemical cycling of actinides, the LLNL BioGeoChemistry of Actinides SFA is performing a combination of field and laboratory studies at Pond B of the Savannah River Site (SRS, South Carolina). Pond B received SRS R reactor cooling water from 1961–1964 that contained trace amounts of Pu (33 MBq ²³⁸Pu and 430 MBq ^{239,240}Pu), ²⁴¹Am, and ¹³⁷Cs (1). Microorganisms are known to interact with actinides through various mechanisms including bioaccumulation, biosorption, bioreduction, and biomineralization. However, little is understood about the influence of extracellular microbial metabolites (exudates) beyond a few complexing and solubilizing agents (e.g., siderophores, citrate and oxalate) and extracellular electron carriers (e.g., flavins). Microbial exudates play an important role in shaping microbial community structure and function and are likely to impact actinide biogeochemical cycles at Pond B.

Pond B naturally stratifies in the summer and is ideally suited to examining the effects of seasonal anoxia. Previous measurements suggest that during stratification, Pu in the particulate and dissolved fraction of the water column will increase in the anoxic zone, but the mechanism(s) causing mobilization are uncertain (1). Our study will focus on characterizing pond and sediment biogeochemical profiles (including microbial community analyses) to determine the long-term migration behavior of ²³⁹Pu, ²⁴¹Am, and ¹³⁷Cs. With these data, we will test the hypothesis that seasonal anoxia leads to remobilization of Pu from shallow sediments into overlying water due to Fe-oxide reductive dissolution and release of microbial exudates. The microbial community and geochemical parameters will be sampled at select locations with depth and time. Laboratory microcosm experiments will be undertaken, mimicking conditions that enrich for specific metabolic activity, such as iron oxidizers, iron reducers, denitrifiers, and sulfate reducers, and correspond to each layer of the stratified pond: epilimnion, thermocline, and hypolimnion (e.g., light/dark cycles, microaerophilic conditions, and anoxic conditions, respectively). Microbial exudates collected from the microcosms will be exposed to Pu to probe for Pu-exudate complexation and specific exudates of interest will be further characterized. Through the combined field and laboratory studies, we will provide insight into how microbial communities can influence Pu fate and transport via extracellular metabolites.

Reference:

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Subsurface Biogeochemical Research

**Oak Ridge National Laboratory
SBR Science Focus Area**

Poster #22-1

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

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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 assets for future use requires developing a deeper understanding of watershed structure and function. Research findings during Phase I of the Critical Interfaces Scientific Focus Area (SFA) project have led to the realization that transient storage zones (TSZs)—and more specifically, metabolically active transient storage zones (MATSZs)—are hot spots for biogeochemical transformations that can exert a controlling influence on downstream water quality. TSZs are surface and subsurface locations (e.g., hyporheic zones) that delay the downstream flow of water in comparison with the main channel. Over the next three years (Phase II), the project aims *to determine the fundamental mechanisms of and environmental controls on Hg biogeochemical transformations in MATSZs in low-order streams*. A key component of this renewal is to parameterize our biogeochemical modeling framework for predicting Hg transformations in East Fork Poplar Creek (EFPC).

Over the past seven months, the SFA team has (1) initiated a planning effort to conduct a series of reach-scale conservative and reactive tracer experiments in EFPC to estimate the volume of TSZs in support of the field-scale model development activity, (2) gained new insights into the effect of light exposure and seasonal changes on Hg transformations in periphyton biofilms, (3) refined our previously developed kinetic model that accounts for changes in Hg bioavailability, and (4) identified a novel Hg stable isotope fractionation mechanism. Additionally, the SFA team is developing new techniques for isolating novel Hg methylators from EFPC microbial communities and gaining new insights into the function of HgcAB proteins using a range of techniques. These include monitoring the growth and metabolite profiles from mutant strains of *Desulfovibrio desulfuricans* ND132 (our model organism), demonstrating that ND132 cell lysates can irreversibly convert mercuric Hg to methylmercury, and predicting the structure of the HgcAB complex using metagenomic sequence analyses. Collectively, these efforts are allowing us to gain a deeper understanding of Hg transformations in EFPC. Although Hg and the EFPC watershed serve as representative use cases, the information generated, and the integrated multiscale approach pioneered by ORNL, will yield a transformational paradigm for integrating an understanding of biogeochemical processes operating in MATSZs into a framework that enables more accurate predictions of water quality at the scale of individual stream reaches and small watershed catchments.

Poster #22-2

Coupled Investigation of Hyporheic Transport and Transformation Dynamics in Headwater Streams: Preliminary Findings and Experimental Design

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Improving the representation of key hydrological processes, such as evapotranspiration (ET), that influence discharge and exchange fluxes in streams is essential to developing a more robust predictive understanding of mercury cycling in low-order streams globally. For example, ET on hillslopes can cause discharge in low-order streams to fluctuate on a diurnal basis. At certain locations and times, the net result can produce spatially intermittent stream discharge— specifically the diurnal presence or absence of surface discharge along a fixed study reach. We expect ET-driven (de)activations of stream flow, more generally, the diurnal variation in hydraulic gradients that link the stream and subsurface, to alter exchange fluxes and transit times along a stream reach. These alterations would result from changes in the geometry of some flow paths, including (de)activation, and changes in the relative flux along flow paths that do not change over time. Variations should both be continuous as discharge rises and falls in response to ET, and exhibit threshold behavior as the stream and/or subsurface pathways activate and deactivate. Associated with these changes, a number of other system states fluctuate on a diurnal basis, including changes in exchange flux, reach scale transit times, and locations oscillating between saturated and unsaturated. Given the changes in both biogeochemical forcing (e.g., saturated to unsaturated conditions) and physical transport (e.g., changing timescales and relative fluxes along flow paths, activation of new flow paths) we expect diurnal variation will be observable in reach-scale ecosystem function, including respiration and nutrient spiraling. We present results of a series of four injections of both conservative and reactive tracers along a study reach with diurnal fluctuations in discharge, including two locations where flow is completely subsurface along the stream. We interpret physical transport by analyzing conservative solute tracer breakthrough curves using both time-series analyses and fitting of a time-variable StorAge Selection (SAS) function; and we infer ecosystem function using resazurin-to-resorufin transformation rates (both modeled and based on field observations).

Finally, we generalize our findings as a series of challenges facing existing and emerging models of transport and transformation in the river corridor. We conclude with a proposed experimental design to measure the spatially heterogeneous and time-varying reactive transport relationships that were identified in our field campaign.

Poster #22-3

Ecosystem Controls on Methylmercury Production by Periphyton Biofilms in a Contaminated Freshwater Stream

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Anthropogenic activities have disrupted the natural mercury (Hg) cycle, releasing large amounts of this naturally occurring toxic element. The neurotoxin monomethylmercury (MMHg) is rarely a direct pollutant; rather, it is formed in the environment by a microbially mediated process known as mercury methylation. MMHg can also be demethylated via biotic and abiotic processes. Monomethylmercury (MMHg) produced by periphyton biofilms represents a substantial fraction of the overall MMHg flux in East Fork Poplar Creek (EFPC), an industrially contaminated creek in Oak Ridge, Tennessee (Olsen et al., 2016); but the environmental factors controlling MMHg production in biofilms are poorly understood. In this study, we used Hg stable isotopes to determine periphyton MMHg production rates across four seasons, two EFPC locations, and two light conditions. Mercury-201 and MM²⁰²Hg were added to intact periphyton samples from EFPC, and the formation of MM²⁰¹Hg and loss of MM²⁰²Hg were monitored over time. These data were used to calculate methylation and demethylation rate potentials using a transient availability kinetic model (Olsen et al., 2018). For methylation, light exposure and season were significant predictors of rate potential, with greater methylation rate potential in full light exposure and in the summer. For demethylation, season, light exposure, and location were all significant predictors of rate potential. Demethylation rate potentials were highest in dark conditions, in the spring, and at the upstream location (closer to the Hg-contamination source). Net MMHg production, the difference between methylation and demethylation, was driven by light exposure, with positive production occurring in periphyton grown under full light exposure and net loss of MMHg occurring in periphyton grown in the dark. On average, transient availability rate potentials were 15× higher and 9× higher for methylation and demethylation, respectively, compared with first-order rate potentials calculated at 1d. Our data show that light exposure is the controlling factor of periphyton net MMHg production in EFPC, and our results underscore the importance of applying transient availability kinetics to MMHg production data to obtain accurate estimates of MMHg production potential and flux.

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Olsen, T.A., Brandt, C.C. and Brooks, S.C. (2016) Periphyton Biofilms Influence Net Methylmercury Production in an Industrially Contaminated System. *Environ. Sci. Technol.* 50, 10843-10850.

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Poster #22-4

Complex Biogeochemical Mechanisms Controlling Mercury Species Transformation and Methylmercury Production in the Environment

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The overall goal of this research is to understand complex biogeochemical processes and interactions between mercury (Hg) and microbes, naturally dissolved organic matter (DOM), particulate organic matter, and minerals in influencing Hg species transformation and availability for microbial uptake and methylation. Using *D. desulfuricans* ND132 as a model methylating organism, we first examined the dynamics of concurrent Hg sorption, uptake, and methylation to resolve whether cells take up Hg passively or actively. We found that, in the absence of thiols, >60% of the added Hg was taken up passively in 48 h by both live and heat-killed cells, as well as cells treated with the proton gradient uncoupler, carbonyl cyanide *m*-chlorophenyl hydrazone (CCCP). Heat treatment or CCCP treatment halted Hg methylation, but it did not stop cellular Hg uptake. Similarly, treatment with CCCP impaired the ability of spheroplasts to methylate Hg but did not stop Hg uptake. Our results indicate that cellular Hg uptake is primarily controlled by Hg speciation and ligand exchange and is independent of active metabolic processes. We also investigated Hg sorption-desorption characteristics on three organo-coated hematite particles and a Hg-contaminated sediment and evaluated the potential of particulate-bound Hg for microbial methylation. Mercury was found to rapidly adsorb onto particulates; however, the presence of Hg-binding ligands—such as low-molecular-weight thiols and humic acids—resulted in up to 60% of Hg desorption from the Hg-laden hematite particulates, but <6% from the sediment.

Importantly, the particulate-bound Hg was bioavailable for uptake and methylation by ND132 cells, and the methylation rate was 4–10 times higher than the desorption rate of Hg. These results suggest that direct contacts and interactions between particulate-adsorbed Hg and cells likely caused rapid exchange and uptake of Hg by ND132 cells. This observation questions the common notion that sorbed or particulate-bound Hg is unavailable for microbial uptake and suggests important roles for particulates as significant sources of Hg for methylation in the environment. We further examined Hg isotope fractionation during abiotic dark oxidation of dissolved elemental Hg(0) in the presence of thiol compounds and DOM. We observed equilibrium mass-dependent fractionation with enrichment of heavier isotopes in oxidized Hg and a small negative mass-independent fractionation owing to nuclear volume effects. These findings provided additional experimental constraints on interpreting Hg isotope signatures, with important implications for the use of Hg isotope fractionation as a tracer of Hg biogeochemical cycles in nature.

Poster #22-5

Microbial Mercury Methylators in East Fork Poplar Creek: From the Field to the Laboratory

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Mercury methylation in the East Fork Poplar creek (EFPC) is primarily a result of microbial biotransformation both in sediments and in periphytic communities. Based on laboratory studies, mercury methylation is conducted by bacteria and archaea that harbor the *hgcAB* genes and that belong primarily to the Deltaproteobacteria, Firmicutes, and Methanomicrobia groups. Previous sequence studies of EFPC communities have identified the presence of potential methylators, but so far none has been characterized based on genomic data or isolated in culture from the site. To achieve a comprehensive understanding of the mercury biotransformations in EFPC, the primary organisms that catalyze methylation need to be identified and characterized. The extremely high diversity of the microbial communities where methylation occurs (up to thousands of species) makes that task difficult, as the methylators are a low fraction of the community (<1%).

To gain access to the microbial methylators in sediments and periphytic communities, we are developing fractionation techniques (e.g., gradient centrifugation) to separate bacteria and archaea from other biotic and abiotic components of the environmental samples. We are also applying flow cytometric fractionation of the complex EFPC microbial communities, based on various cellular characteristics including size and morphology, as well as labeling with antibodies raised against cultured bacteria and archaea that methylate mercury. Populations of cells enriched for methylators will be characterized by metagenomic sequencing and will also be used for laboratory enrichments to isolate and characterize novel Hg methylators.

In parallel, we are conducting laboratory experiments aimed at characterizing the interaction of known bacterial and archaeal methylators and how environmental factors impact methylation rates. Species related to those found in EFPC are being grown under steady state conditions in single cultures and in increasingly complex co-cultures to measure cell counts, Hg methylation rates, electron donors and acceptors, organic acids, H₂ and CO₂ concentrations, carbon balancing, and gene expression levels. The selected strains represent different anaerobic functional groups (iron and sulfate reduction, fermentation, syntrophy, methanogenesis), allowing us to directly characterize the phenotypic effects of multi-species interactions on Hg- methylation and cellular metabolism. Methylating organisms isolated from EFPC will ultimately be integrated in these studies and used to identify general and EFPC-specific metabolic and Hg biotransformation characteristics. Ultimately, the outcomes of these studies will further inform modeling of mercury biogeochemical processes in EFPC.

Biomolecular Processes Contributing to Hg Transformations at Critical Interfaces

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Mercury (Hg) methylation is an enzyme-catalyzed process associated with the activity of anaerobic bacteria and archaea carrying the *hgcAB* gene cluster. We determined the kinetics of enzymatic Hg methylation in cell lysates of the model Hg-methylating bacterium *Desulfovibrio desulfuricans* ND132 and demonstrated that the activity of the proteins HgcA and HgcB irreversibly converts mercuric Hg (Hg(II)) to methylmercury (MeHg). The chemical speciation of the Hg(II) substrate is an important factor to consider because of the high affinity of Hg(II) for biological thiols with stability constants of up to 45 for Hg(II)-bis-thiolate complexes, which may limit the availability of Hg(II). We investigated the impact of thiol levels on MeHg formation by HgcA and HgcB and found that methylation activity is not impaired at high thiol/Hg(II) ratios. Furthermore, we explored the roles of cellular metabolites in Hg methylation activity in ND132 cell lysates. We identified a dependence between S-adenosyl methionine levels and Hg methylation rates. The results provide new insights into the function of HgcA and HgcB and their interdependence with cellular metabolism.

Methanotrophs expressing the copper-chelating compound and chalkophore methanobactin can bind and demethylate MeHg, potentially limiting the net production of MeHg in the environment. Initial studies investigated the prevalence of methanotrophs and Hg-resistant bacteria in East Fork Poplar Creek (EFPC) by analyzing metagenomic data for biomarkers of methanotrophs and the prevalence and diversity of Mbn gene clusters, which are essential for the expression of methanobactins. Furthermore, we analyzed methanobactin precursor sequences (*mbnA*) and identified a set of methanobactins potentially present in EFPC. The overall goal is to assess the role of methanotrophic-mediated Hg detoxification among the broader microbial community in EFPC.

Poster #22-7

A Multi-Pronged Approach to Identifying the Biochemical Function of Hg Methylation Proteins in *Desulfovibrio desulfuricans* ND132

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Methylmercury (MeHg), an organic mercury (Hg) compound, is a potent toxin that bioaccumulates in food sources and is primarily produced by microorganisms in anaerobic organic-rich soils and sediments. A persistent challenge in studying environmental MeHg production is understanding how and why microbes produce the toxin. To date, little is understood about the physiological function of MeHg production by anaerobic microorganisms. It is postulated that the native function of the Hg methylation proteins (HgcAB) is not Hg methylation, but rather the methylation of an unknown metabolite. Mercury methylation has been linked to C1 carbon metabolism for acetyl-CoA and methionine biosynthesis, sometimes as part of the Wood-Ljungdahl pathway; yet a specific biochemical pathway remains elusive. We are taking a systems biology approach to explore the physiological function of Hg methylation using *Desulfovibrio desulfuricans* ND132 as a model organism. For this study, we compared growth and metabolite profiles of various *D. desulfuricans* ND132 gene deletion strains related to carbon and Hg cycling with those of the wild-type strain. Mutant strains (e.g., $\Delta hgcAB$, $\Delta metH$, $\Delta cobT$, $\Delta hgcA:T101A$) that exhibited differences in Hg methylation capability compared with wild-types (e.g., 0–246%) were grown in defined media with various substrates (e.g., pyruvate, fumarate, lactate, sulfate, formate, acetate). Organic acid, anion, and metabolite concentrations were monitored throughout the growth of the cells to determine if changes in central metabolism coordinated to changes in MeHg generation between wild-type and mutant strains. Indeed, significant differences in substrate consumption, acetate production, and transcription of C1 metabolism genes were observed between the strains under fermentative and sulfate-reducing conditions. To further elucidate the native contribution of HgcAB to cellular metabolism, *D. desulfuricans* ND132 wild-type and $\Delta hgcAB$ cultures were grown together with various substrates to measure the epistatic fitness effects of deleting *hgcAB* under relevant environmental conditions. Identifying the conditions under which *hgcAB* provides a fitness benefit will aid in identifying other functions for this enzyme.

Poster #22-8

Structure Determination of the HgcAB Complex Using Metagenome Sequence Data

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Bacteria and archaea possessing the *hgcAB* gene pair can methylate inorganic mercury to form highly toxic methylmercury. Previous sequence analyses revealed that HgcA consists of a corrinoid binding domain and a transmembrane domain, and HgcB is a ferredoxin with two 4[Fe-4S] clusters. However, the detailed structure and function of these proteins are not well understood. Recent advances have enabled highly accurate structural models of proteins to be generated by combining metagenome sequence data, coevolution analysis, and ab initio structure calculations. We use this approach to generate a complete structural model of the assembled HgcAB complex. The model confirms many previously predicted structural features and reveals new insights into the structure and function of these two proteins. Surprisingly, the coevolution analysis revealed that the two domains of HgcA do not interact with each other, but HgcB binds to both of these domains in the assembled complex. In addition, there is evidence for dynamic movement of individual domains relative to each other, which likely plays an important role in methyl transfer. These findings expand the repertoire of known corrinoid methyltransferase folds, provide structural and mechanistic insight, and form the basis for identifying additional proteins involved in mercury methylation.

Subsurface Biogeochemical Research

**Pacific Northwest National Laboratory
SBR Science Focus Area**

Pacific Northwest National Laboratory SFA: Influences of Hydrologic Exchange Flows on River Corridor and Watershed Biogeochemical Function

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The PNNL SFA is developing predictive understanding of processes that govern influences of hydrologic exchange flows on water quality, nutrient dynamics, and ecosystem health in dynamic river corridor and watershed systems. Exchange of water between rivers and subsurface environments (hydrologic exchange flows or HEFs) are a vital aspect of watershed function.

HEFs enhance biogeochemical activity and modulate water temperatures, thus playing a key role in water quality, nutrient dynamics, and ecosystem health. However, these complex processes are not well understood in the context of large managed rivers with highly variable discharge, and are poorly represented in system-scale quantitative models. The PNNL SFA is studying the biogeochemical and ecological impacts of hydrologic exchange flows and their cumulative impacts at reach to watershed scales. Using the 70-km Hanford Reach of the Columbia River as our primary research domain, the project emphasizes three integrated elements:

1. *Development of fundamental understanding of the effects of river dynamics and organic carbon character on biogeochemical processes.* We performed laboratory and field studies, including development of new sensor technologies, to characterize organic matter in diverse river systems and understand its impact on biogeochemical and ecological processes. We developed the WHONDRS network as an exemplar of community science to extend understanding beyond our own testbed site.
2. *Incorporation of new understanding into mechanistic models of coupled hydrologic and biogeochemical processes in the river corridor.* We constructed new biogeochemical networks based on metagenomic and metabolomic information. We developed and tested a framework for modeling coupled river-subsurface processes, then applied it to a 7-km segment of the Hanford Reach encompassing multiple hydromorphic classes to quantify residence time distributions.
3. *Use of mechanistic models to develop reduced-order representations of the function of large-scale systems (reach to watershed) with emphasis on interactions between energy, water, and ecological subsystems.* We developed a reach-scale (70-km) model of subsurface flow linked to river stage variations and used it to study spatiotemporal variations in HEFs and temperature. We have used field observations and coupled subsurface-land surface models to evaluate the impacts of HEFs on land surface fluxes (e.g., through eddy covariance stations that recently joined the AmeriFlux network). We are also developing new field observations including geophysical sensing of riverbed characteristics and water quality monitoring, and have assimilated field observations into reach- and watershed-scale models to quantify cumulative impacts of local processes on watershed function.

Understanding Influences of Hydrologic Exchange Flows on River Corridor Function in a Managed Watershed through Integrated Modeling and Observations

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This element of the PNNL SFA is monitoring key components that modulate carbon and nitrogen dynamics along the river corridor of a managed watershed and employing results in a novel watershed modeling framework with explicit representations of river corridor processes. Hydrologic exchange increases contact time with reactive environments within river corridors (RCs), facilitating biogeochemical reactions and controlling the fate and transport of solutes along the river corridor, and therefore impacting ecosystem health and responses to changing hydro-dynamic conditions.

Our watershed modeling framework features the coupling among PFLOTRAN, a massively parallel subsurface reactive transport model, the Community Land Model (CLM), and the river routing model from the Soil and Water Assessment Tool (SWATR). As a proof-of-concept, we apply the modeling framework in the Upper Columbia-Priest Rapids (UCPR) watershed to investigate the influence of RC on watershed function. Long-term observations from three eddy covariance stations as part of the AmeriFlux network, groundwater monitoring well, and discharge from USGS streamflow gages were used to inform and validate the model. Our results show that the upland and riparian ecosystems exhibit drastically different water and carbon dynamics. The upland sagebrush-steppe ecosystem relies heavily on rainfall for water supply, and ET and NEE peak in late spring when both precipitation and energy inputs are relatively high. In contrast, the riparian sagebrush-steppe and grassland ecosystems are dominated by exchanges between river water and groundwater, and ET and NEE peak in the summer when plants are physiologically active and less water-stressed.

To investigate the effect of hydrological exchange and biogeochemical processes on the fate of nutrients, SWATR has been enhanced with a multi-rate mass transfer (MRMT) module, created to model the coupled nonlinear multicomponent reactive transport in the channel water and its surrounding RCs. RCs are conceptualized as transient storage zones where two-step denitrification and aerobic respiration reaction are represented. By applying the SWATR-MRMT model to the UCPR watershed with estimated transfer rates with the basin-scale Networks with EXchange and Subsurface Storage (NEXSS) model, our simulation results suggest that (1) only biogeochemically active vertical RCs can contribute to significant nitrate removal in surface water due to the short residence times; and (2) mass transfer using a single exchange rate rather than a spectrum of exchange rates may overestimate the attenuation role of RCs.

Future work in improving the coupling among model components and collecting additional observations to inform and validate the model will be discussed.

Reach-Scale Hydrologic Exchange Flows and Their Impacts on Hyporheic Thermal Regimes

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This element of the PNNL SFA seeks to study the effects of river morphology and sediment permeability on river corridor hydrologic exchange flows (HEFs) and seasonal thermal dynamics under hydropeaking and thermopeaking. Water temperature in the hyporheic zone can powerfully impact river biogeochemistry and ecology through, for example, controls on dissolved oxygen levels supporting fish health or modification of microbial reaction rates. We have previously shown that HEFs strongly control hyporheic zone temperature in local domains. To extend this knowledge to larger scales, we developed a 3-D numerical model using PFLOTRAN for a large (75-km) regulated river corridor of the Hanford Reach. This model was used to evaluate the impacts of dam-regulated flow conditions and hydrogeomorphic features on HEFs, the associated river corridor thermal regime, and its implications for river ecology. Our results revealed highly variable intra-annual spatiotemporal patterns in HEFs along the reach, as well as strong interannual variability with larger exchange volumes in wet years than dry years. The magnitude and timing of river stage fluctuations controlled the timing of high exchange rates. Both river channel geomorphology and the thickness of a highly permeable river bank geologic layer controlled the locations of exchange hot spots, while the latter played a dominant role.

River corridor thermal regime was strongly influenced by high-frequency flow variations interacting with river temperature dynamics. As HEFs exhibit hot spots and hot moments, so also river corridor thermal regime exhibited strong spatiotemporal variability. Riverbed temperature lagged behind surface water temperature and the amplitude of riverbed temperature fluctuations was ~60% less as compared to that of surface river temperature. Riverbed morphology such as islands and gravel bars created areas of upwelling and downwelling that affected the penetration depth of the thermal signal. In general, thermal signals penetrated deeper at the upstream end of morphologic features where strong downwelling occurred. Thermal signals also penetrated deeper where highly permeable sediments existed causing larger exchange flux, creating colder zones in the winter and warmer zones in the summer. These simulated changes in river corridor thermal regime would impact the selection of the spawning area by salmonids and their survival rate. Our results demonstrated that upstream dam operations enhanced the exchange between surface water and groundwater and changed river corridor thermal regime with strong potential influence on river ecology.

Mechanistic Models of Hydrologic Exchange Flows in Diverse Hydromorphic Settings

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This element of the PNNL SFA seeks to develop mechanistic understanding of hydrologic exchange flows (HEFs) and associated biogeochemical processes and develop approaches for representing these processes at system scales.

Hydrologic exchange between rivers and subsurface environments is a critical mechanism that shapes hydrobiogeochemical processes in river corridors and watersheds. Because of limitations in field accessibility, computational demand, and complexities of geomorphology and subsurface geology, three-dimensional mechanistic modeling studies to quantify hydrologic exchange flows (HEFs) have been mostly limited to local-scale applications in individual bedforms. Although it is well known that surface flow conditions, riverbed morphology, and subsurface physical properties strongly modulate hydrologic exchanges, quantitative measures of their effects on the strength and direction of such exchanges in complex hydromorphic settings are lacking.

Here, three-dimensional models of coupled river hydrodynamics and subsurface flow and transport simulations in diverse hydromorphic settings are used to study the hydrologic exchange flows and residence time distributions at kilometer scales in order to support the development of reduced-order models at reach and watershed scales. Hydrologic exchange is often simulated by assuming hydrostatic pressure on the river bed as a boundary condition. In this study, the impact to HEFs driven by the non-hydrostatic pressure variations on the riverbed are explored by comparing model results simulated by PFLOTRAN (an open source subsurface flow and transport model) driven by 1) non-hydrostatic pressure simulated using open-source computational fluid dynamics (CFD) software OpenFOAM, and 2) hydrostatic pressure simulated by the 2D Modular Aquatic Simulation System (MASS2) model. Particle tracking is used to quantify residence time distributions (RTDs) within a 7-km river section at the Hanford 100FH area. Model outputs are analyzed in the context of classes of hydromorphic features (previously defined and mapped over the entire Hanford Reach) to quantify the impacts of hydromorphology on HEFs and RTDs for each hydromorphic class. This new understanding is guiding development of reduced-order modeling at reach to watershed scales and the selection of locations for field studies.

Poster #21-71

Metabolic Network and Multi-omics Integration for Predictive Biogeochemical Modeling

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This element of the PNNL SFA seeks to improve predictive biogeochemical process modeling through incorporation of the microbial control exerted on biogeochemical dynamics. Current models that take a reductionist approach provide a monolithic description of microbial processes, largely due to the difficulty in characterizing the complex communities. Rapid advancement of high-throughput profiling technologies has generated a large body of multi-omics data for environmental systems, addressing this limitation. To link this molecular data with biogeochemical and ecosystem models across scales, modeling frameworks that can fully take advantage of those unprecedented resources must be developed. Here, we present genome-scale metabolic networks as an ideal tool to fill this gap. While metabolic network modeling has been commonly used for studying single organisms growing in well-defined media, its application to complex environmental microbial systems poses several challenges to overcome as described below. By leveraging the DOE's KBase (<https://kbase.us/>) modeling and chemoinformatics tools, we propose new pipelines and workflows that enable network reconstruction and data integration for environmental systems to inform biogeochemical models.

First, we developed a new approach to construct metabolic networks from metagenomes. This is challenging in general due to the volume and complexity of metagenome data. As a key idea to address this issue, we reduced data handling by storing only identified activities and metadata such as their counts and estimated taxonomic origin, not all predicted genes. Subsequently, we applied this network reconstruction method to field metagenome data to model microbial communities sampled from two riverbank sediments with and without vegetation. Through a comparative analysis of the two constructed metabolic networks, we were able to identify metabolic pathways 1) that can uniquely characterize biochemical reactions pertaining to each site and 2) that are found in common at two sites. While this result demonstrates the capability of our approach that differentiates biogeochemical traits between two sites, metagenome-based networks could not capture all key differences as indicated by metabolite profiles obtained from FTICR-MS. Thus, we further developed a method to incorporate high-resolution metabolite profiles into metabolic networks. The resulting metabolite-informed networks provide a better representation of functional characteristics of the systems. This new development will significantly be expanded using metabolite data from WHONDRS, a global consortium led by the PNNL SFA to broadly study hydro-biogeochemical function of river corridors. As an important next step, we are undertaking efforts to integrate these new metabolic networks into reactive transport models through collaboration with the IDEAS project.

Poster #21-72

Field Observations of Hydrologic Exchange Flows and Biogeochemical Impacts

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This element of the PNNL SFA seeks to gain new understanding of coupled hydrologic and biogeochemical processes in the hyporheic zone through novel instrumentation linked to numerical models. Quantifying the spatial and temporal pattern of hyporheic respiration remains a key gap in field studies as well as river reach-scale reactive transport modeling. Accurate simulation and prediction biogeochemical function within the hyporheic zone (HZ) of dynamic, regulated river systems is dependent on corresponding understanding of the distribution of physical properties that govern hydrologic exchange fluxes (HEFs) and the metabolic reactions that take place within the HZ. To better inform coupled hydrological and biogeochemical models of HZ function, we are developing novel tools and analytic techniques that enable simultaneous monitoring of dynamic fluxes and HZ respiration rates: the flux tool and the optode-based oxygen sensor.

The flux tool consists of a vertical array of sensors deployed in the riverbed. The sensors record time series of pressure gradient, temperature, fluid electrical conductivity, and bulk electrical conductivity. Collectively, these time series provide adequate information to estimate the vertical distribution of porosity and permeability using a companion high-performance hydrogeophysical joint inversion software. Once the system is 'calibrated' using the flux tool and software, the tool is removed and long term monitoring of dynamic flux is accomplished using only dynamic pressure, temperature, or fluid conductivity measurements.

Dynamic river flows lead to HZ conditions that vary the ratio between oxygen consumption and resupply in reactive transport models. Understanding these coupled flow and biogeochemical processes requires knowledge of both reaction and transport timescales. The flux tool provides the flow physics half of this equation, but existing methods for measuring in-situ HZ respiration are inadequate. To fully link hydrology and biogeochemistry, we require a sensor able to measure oxygen concentrations in the HZ at high spatial and temporal resolution. Previous work has shown limited success using off the shelf fiberoptic oxygen sensors combined with custom optode-coated tubes. We pursue that avenue, while simultaneously developing a more robust and compact system with no moving parts to measure and log a linear profile of oxygen concentration. Using these tools together, we test the hypothesis that the evolution of the oxygen profile will lag behind perturbations in vertical flux, leading to complex responses in highly dynamic rivers. Understanding these interactions is critical to properly parameterizing large-scale GW/SW interaction models.

Poster #21-73

Spatiotemporal Variation in Organic Matter Chemistry in Global Rivers Modulates Biogeochemistry

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This element of the PNNL SFA seeks to understand spatiotemporal variation in organic carbon chemistry and its influences on river corridor biogeochemical function. Dissolved organic matter (DOM) chemistry is emerging as a strong influence on biogeochemical cycling in river corridors. However, reactive transport models do not currently consider chemical properties of DOM, indicating a significant structural gap that limits our ability to predict integrated hydro-biogeochemical function. To enable the incorporation of DOM chemistry into reactive transport models, we are (1) characterizing spatiotemporal patterns in DOM chemistry, (2) revealing mechanisms that underlie subsequent influences on river corridor biogeochemistry, and (3) developing new representations of DOM chemistry that can be incorporated into numerical models.

We present integrated research that addresses spatiotemporal characterization, mechanistic insight, and model representation of DOM in river corridors. We established a global research consortium (WHONDRS) to advance cross-system characterization of patterns in DOM chemistry and integrated hydro-biogeochemical function of river corridors. One WHONDRS effort characterizes temporal dynamics of DOM in surface and pore water under sustained high-frequency river stage fluctuations. Using new cheminformatics approaches inspired by ecological theory, this effort is revealing the spatiotemporal organization of model-relevant attributes of DOM chemistry and their relationship to biogeochemical dynamics. To evaluate the mechanisms underlying biogeochemical impacts of DOM chemistry, we paired laboratory experiments with new biogeochemical modeling approaches that account for thermodynamic and microbial regulation of respiration. Aerobic sediment slurries revealed that transitioning from C-limited to C-replete conditions was associated with a transition from thermodynamic regulation of respiration to limitation by organic N. These results point to interactions among thermodynamics, C concentration, and organic N availability as key controls on respiration rates in river corridors. In addition, these results challenge classical theory that discounts the relevance of DOM thermodynamics under aerobic conditions. To better understand the contradiction between theory and experimental outcomes we developed a numerical model to investigate the biogeochemical role of DOM chemistry in aerobic environments. The model revealed that thermodynamically favorable DOM promotes mineralization of less favorable DOM. Model outcomes therefore provide additional support to the inference that thermodynamic properties of DOM influence biogeochemical rates under aerobic conditions. This suggests the need to reconsider classic theory and revise models accordingly. Collectively, we are providing the data, field instrumentation, mechanistic knowledge, and theory to integrate DOM chemistry with hydrology to enhance predictive understanding of hydro-biogeochemical function in river corridors.

Poster #21-74

Exploring the Synchrony of Hydrologic Exchange Processes Along River Corridors

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This element of the PNNL SFA seeks to understand and quantify the hydrologic connectivity of river corridors by studying relationships among river channels, hyporheic zones, floodplains and ponded waters and their relative roles in hydrologic exchange. Mechanistic understanding of watershed and river corridor processes is critical for modeling and prediction and to sustainably manage water resources under present and future socio-economic and climatic conditions. In this work, we used the model Networks with EXchange and Subsurface Storage (NEXSS) to assess when and where different hydrologic exchange processes are active along rivers within the continental United States. In particular, we investigate the synchrony of exchange between river channels and their adjacent hyporheic zone, floodplain, and ponded waters. Synchrony is expected to amplify the biogeochemical effects of river corridor connectivity, resulting in a dominant control for water quality at the local and watershed scales. Asynchrony, on the other hand, is expected to attenuate the effects of connectivity. Using a simple routing scheme, we translate NEXSS estimates of fluxes and residence times into a cumulative measure of river corridor connectivity at the watershed scale, differentiating the contributions of hyporheic zones, floodplains, and ponded waters. We find that the relative role of these exchange subsystems changes seasonally, driven by the intra-seasonal variability of discharge. We also find that the interplay between exchange processes varies with location, typically characterized by asynchrony in low-order streams and synchrony in high-order rivers. Understanding the competing nature of exchange processes is critical to represent connectivity in physics-based models for water quality and to design, implement, and evaluate sustainable water management practices at the scale of the nation.

Subsurface Biogeochemical Research

SLAC

SBR Science Focus Area

Poster #22-22

SLAC Groundwater Quality SFA: Modeling and Scaling of Biogeochemical Responses to Hydrologic Transitions in Floodplain Aquifers

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Alluvial aquifers exhibit complex geological structures such as fine-grained sediment lenses, owing to their depositional and post-depositional histories. These features translate into highly variable hydraulic and geochemical properties that mediate subsurface and surface water quality. In the U.S. intermountain West, large shifts in hydrologic conditions associated with seasonal snowmelt additionally trigger important fluctuations in the biogeochemical functions of alluvial aquifers, which are strongly influenced by these subsurface structures. Recent studies have pointed out that fine-grained, organic-enriched sediments (*i.e.* naturally reduced zones, NRZs, and transiently reduced zones, TRZs) can exert outsized control on groundwater geochemistry because their large inventories of C, S, and Fe, as well as contaminants like U, Mo, Zn, and Pb, can be released by diffusion into the advective zones (AZs) of the aquifer during water table fluctuations that alternately deliver oxygen-rich water to the system or create reducing conditions. In spite of the importance of NRZs and TRZs, there is much that we don't know about rates of reactions occurring within and the various mechanisms of coupling between abiotic and biotic processes and between biogeochemical processes and hydrologic changes that trigger redox and groundwater quality responses.

Here we develop detailed reactive transport simulations of a contaminated alluvial aquifer system at a DOE legacy uranium ore-processing plant in the Wind River Basin near Riverton, WY. By explicitly accounting for N, C, Fe, S and U cycling across the AZ-NRZ interface at the scale of a single NRZ, we evaluate the fundamental processes that control the transfer of elements to and from AZs, including the biogeochemical network, the relative length scales, and the physical and chemical properties of the porous media. We aim at a systematic simplification of the functioning of NRZs that could be integrated into larger scale models, for instance by linking spatial and temporal variability through the use of characteristic transport and reaction timescales. Such an approach could allow for large-scale simulations of water quality, ideally in combination with highly resolved reactive transport simulations.

Poster #22-21

SLAC Groundwater Quality SFA: Biogeochemical Redox Responses of Soil Microbial Communities to Seasonal Hydrological Transitions at Riverton, WY

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The subsurface capillary fringe is a hotspot for biogeochemical cycling and microbial metabolic activity in soils, particularly those in alluvial systems. At the DOE legacy uranium ore processing site in Riverton, WY, extensive seasonal and episodic wet-dry cycling produces intense water table fluctuations that trigger strong redox oscillations throughout the soil column and large variations in dissolved uranium concentrations. Coupling between subsurface hydrology and biogeochemistry is most complex at unsaturated-saturated interfaces, due to the many hydrologic processes at play (percolation, capillary rise, advection) and the biogeochemical reactions that can be triggered (redox reactions, mineral dissolution and precipitation, sorption and desorption, etc.). The intense, intermittent hydrologic transitions and their biogeochemical consequences are governed in large part by the microbial response, which is then responsible for ensuing impacts on groundwater quality, including contaminant release and transport. How exactly the various microbial and geochemical processes are connected in non-steady state, spatially-heterogeneous systems is not yet understood.

We aimed to address this knowledge gap by collecting both microbial and geochemical samples to capture key redox transitions at the Riverton site from April to September 2017. Our goal was to characterize the microbial community throughout the soil column and observe its response to wet-dry transitions across a complete season. Next-generation sequencing (Illumina) was employed to identify biogeochemically-relevant microbial taxa based on the 16S rRNA gene, and also facilitated the identification of key samples for metagenomic and metatranscriptomic sequencing. We found a broad diversity of microbial clades in our samples, including bacteria involved in sulfur oxidation or reduction, dissimilatory metal-reducing bacteria, and ammonia-oxidizing Archaea. Overall, microbial communities grouped by soil depth or type. These data were paired with measurements of major biogeochemical elements (C, N, Fe, S) and metal contaminants (U, Mo), as well as soil temperature and moisture. Together, these results provide insight into how microorganisms respond to hydrologic transitions, and whether they are present and active during both wet (reducing) and dry (oxidizing) periods or only when conditions are optimal for their metabolism. This information is crucial for our understanding of these environments and we will apply these data to enhance reactive transport models capable of testing sensitivity of alluvial systems to hydrologic perturbations.

Poster #22-19

SLAC Groundwater Quality SFA: Impact of Reduced Zones and Hydrological-Biogeochemical Coupling on Solute Transport and Groundwater Quality

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Floodplain water quality is mediated by large seasonal changes in sediment water saturation, redox status, and the extent to which sediments interact and exchange solutes with groundwater. Strong spatial and temporal heterogeneities help mediate the availability and transport of redox active contaminants. For example, it has been postulated that inflow of oxygenated water into naturally reduced zones (NRZs) would stimulate oxidative release of U. However, recent laboratory experiments and field investigations suggest that oxygenation of groundwater can also lead to attenuation of U. In spite of their importance, the mechanisms and resilience of this effect have not yet been fully elucidated. Here we examine hydro-biogeochemical interactions to establish mechanistic controls over water quality in sediments experiencing influxes of oxygen.

In a dual domain column experiment, we used coarse grained aquifer material from the Riverton, WY, field site and inserted a varying number (0-3) of small spherical NRZs with elevated U concentrations and a natural background abundance of As. Oxygenated groundwater (without U for the first 8 weeks, then with U) was pumped through the columns and depth resolved pore water data was collected from inside NRZs and between them. Although we observed U loss from all NRZs, the same amount (or more) of U was retained in the aquifer material. This was attributed to sulfidic conditions having spread into the coarse-grained material around each NRZ. Consequently, Fe(II), As, and sulfides entered the groundwater around each NRZ, whereas U concentrations decreased with each NRZ encountered along the flow path. We conclude that high concentrations of sulfate in Riverton groundwater, together with the presence of soluble organic carbon in NRZs, sustained sulfate reduction inside NRZs; sulfide diffusion into the groundwater then drove oxygen consumption and reduction of Fe, As, and U. Thus, even small scale redox interfaces in S rich environments can strongly alter groundwater quality.

Another sulfide-bearing system experiencing strong redox fluctuations is the Pb- and Zn-contaminated alluvium along Slate River, CO. Seasonal (summer-fall 2018) measurements of dissolved solutes in pore water indicated strong variability that correlated with soil moisture content (and hence, oxygenation). Fe(II) concentrations declined more than 100-fold, while Zn increased more than 10-fold between moist (early-June) and dry (mid-August) conditions. X-ray microprobe analysis and X-ray absorption spectroscopy of Pb, Zn, and S showed that Pb and Zn are hosted by sulfide, Fe-oxide, and clay minerals, depending on depth and redox status, and that there is a strong vertical redox gradient. These results partially confirm our initial hypothesis that oxidative dissolution of sulfides drives the release of Zn, other metals, and organic carbon, thereby mediating water quality.

Poster #22-20

SLAC Groundwater Quality SFA: Mechanisms Controlling Colloid Formation and Impact on Water Quality in Alluvial Sediments

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Colloids help mediate the mobility of contaminants and nutrients in alluvial sediments that experience strong wet-dry redox cycling, which are common at SBR research sites. Here, we will present data suggesting that a large fraction of dissolved organic carbon in the saturated zone in alluvium along the Slate River, Gunnison Co, CO occurs is associated with iron sulfide colloids. Significantly, however, there are large gaps in our understanding of the nature of these colloids and parameters controlling their generation. In this study, we hypothesized that, during hydrological-redox transitions, oxidation of dissolved sulfides (onset of oxidizing conditions) or reductive dissolution of goethite and ferrihydrite (reducing conditions), releases organic carbon, metals, and anions, providing conditions ideal to generate colloids that can bind and mobilize U, Mo, Zn, and Pb. These are important alluvial contaminants at the Riverton, WY DOE legacy uranium ore processing site and at Slate River, within the LBNL Watershed Function SFA study domain. Knowledge of colloid formation and metal binding is needed to improve our understanding of how water quality will respond to hydrological changes such as drought and flooding.

Here, we examined the influence of sulfidation of Fe^{III}-(oxyhydr)oxides nanoparticles associated with organic ligands on the generation, stability, and nature of colloids. We observed that reductive dissolution of ferrihydrite generated nanocluster colloids of mackinawite (FeS). Their subsequent aggregation, which promotes settling of mackinawite, was directly correlated to the concentration of sulfides relative to the iron oxides (S/Fe ratio). At low sulfide concentration (S/Fe ratio ≤ 0.5), the aggregation of mackinawite suspended nanoclusters took up to 14 days, indicating that during the first 14 days of sulfidation, colloids are able to bind and transport metals in groundwater. Inversely, at high sulfide concentration (S/Fe ratio > 0.5) the sulfidation rate was rapid and the aggregation of mackinawite nanoclusters was accelerated, preventing generation of stable colloids. The presence of organic ligands can increase the time of residence of stable nanocluster colloids. The S/Fe ratio also controlled the concentration of DOC, which dramatically increased at high sulfide concentrations, thus promoting the mobility of organic-bound metals. Consequently, the effect on metal and actinide mobility and groundwater quality by sulfidation is dependent on the affinity of contaminants to bind to organic, Fe^{III}-(oxyhydr)oxide, and mackinawite colloids, as well as the relative concentrations of these different phases. Elevated ionic strength accelerated nanocluster aggregation, inhibiting stable colloid generation. This investigation provides for the first time a general conceptual framework to predict the formation and reactivity of sulfidic nanoparticles in alluvial systems in response to wet-dry cycle perturbations.

Subsurface Biogeochemical Research

IDEAS-Watersheds Project

Poster #22-14

IDEAS-Watersheds: Accelerating Watershed Science through a Community-Driven Software Ecosystem

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Project: IDEAS-Watersheds (LANL)

Project Website: <https://ideas-productivity.org/ideas-watersheds/>

Through its Science Focus Area (SFA) projects the Subsurface and Biogeochemical Research (SBR) program is tightly integrating observations, experiments, and modeling to advance a systems-level understanding of how watersheds function, and to translate that understanding into advanced science-based models of watershed systems. To enhance and broaden the impact of the existing SFAs, the IDEAS-Watersheds project builds on the success of a synergistic family of IDEAS projects initiated in 2014. Specifically, it strives to improve watershed modeling capability by increasing software development productivity - a key aspect of overall scientific productivity - through an agile approach to creating a sustainable, reliable, software ecosystem with interoperable components. In this poster we highlight the overall objectives and structure of the IDEAS-Watersheds project, which is organized around six Research Activities. There are three Partnership Activities, each undertaken jointly with one of SBR's interdisciplinary watershed focused SFA projects using concrete use cases to advance our watershed modeling capability. These projects include the Watershed Function SFA (LBNL - poster by S. Molins), the Critical Interfaces SFA (ORNL - poster by S. Painter), and the River Corridor SFA (PNNL). A Continental United States (CONUS) Activity will advance a basin-to-continental scale simulation platform (poster by L. Condon), and a Reaction Network Activity partnering with SBR's fine-scale SFAs focused on fundamental biogeochemical processes to bring those advances into geochemistry reaction modeling tools (see poster by S. Molins). These projects include the Subsurface Biogeochemistry of Actinides SFA (LLNL), the Wetland Hydrobiogeochemistry SFA (ANL), and the Groundwater Quality SFA (SLAC). Finally, a Shared Infrastructure Activity will coordinate the development of common workflow tools and software interfaces to support interoperability. We adopt a co-funding model with shared deliverables and joint funding of postdocs and SFA-IDEAS liaisons to facilitate training of early career researchers and ensure integration with the SFAs.

As an important example of emerging workflow tools we highlight plans in our partnership with the River Corridor SFA (PNNL) to work with KBase Apps and its Narrative interface. We describe our approach to develop KBase Apps that enable batch and 1D reactive transport model simulations (e.g, with PFLOTRAN) to study the reaction networks being developed through metabolic pathway analyses. This development will establish mechanistic links between metagenomes and biogeochemical modeling, and will also support our collaboration with the Wetland Hydrobiogeochemistry SFA (ANL).

Poster #22-13

IDEAS-Watersheds Partnership with the Critical Interfaces SFA: Progress and Plans

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The next phase of the Interoperable Design of Extreme-scale Application Software project (IDEAS-Watersheds) will focus on development and demonstration of critical modeling capabilities needed to further advance process-rich watershed hydro-biogeochemical models. To help advance that capability, the project has adopted concrete watershed modeling use cases in partnerships with interdisciplinary watershed-focused Science Focus Areas (SFAs). A common modeling challenge for watershed hydro-biogeochemical models is how to tractably represent the effects of processes associated with spatially localized metabolically active transient storage zones. The IDEAS-Watershed partnership activity with the Critical Interfaces SFA is addressing that multiscale modeling challenge using the transport of Hg and its microbially mediated transformation to the neurotoxin methylmercury (MeHg) in East Fork Poplar Creek (EFPC), Tennessee as a use case. The partnership is developing a new multiscale modeling approach (Painter 2018) that extends highly successful residence-time approaches to accommodate nonlinear multicomponent reactions and transient flows. Building on previous capabilities developed by the IDEAS project, the approach has been implemented as a hyporheic-zone subgrid model in the integrated surface/subsurface hydrology code ATS (Coon et al. 2016). A non-reacting tracer test (Ward et al. 2016) at the HJ Andrews Experimental Forest that was strongly affected by transient channel flow has been successfully modeled. We are developing tools to perform parameter estimation from the tracer tests, focusing on hyporheic exchange rates and non-parametric estimation of the hyporheic travel-time distributions. Longer term, we plan to do reach-scale reactive transport demonstration simulations for the HJA Watershed 01 and EFPC, develop interfaces that will allow output of the USGS NEXSS model (Gomez-Velez, 2014) to be ingested into ATS for the purpose of river-basin-scale biogeochemical simulations, and perform river-basin-scale demonstration simulations.

References:

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Poster #22-11

IDEAS-Watersheds: Partnership with the Watershed Function SFA and Fine-Scale Reaction Network Activities

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Project: IDEAS-Watersheds (LBNL)

Project Website: <https://ideas-productivity.org/ideas-watersheds/>

The next phase of the Interoperable Design of Extreme-scale Application Software project (IDEAS-Watersheds) will focus on development and demonstration of modeling capabilities needed to further advance process-rich biogeochemical reaction network models and hydro- biogeochemical watershed models. In this presentation, we will discuss two activities within the project: (1) the partnership with the Watershed Function SFA to develop a multiscale modeling framework that will allow us to consider processes at different resolutions within the watershed and (2) the fine-scale activities in collaboration with the SLAC, ANL and LLNL SFAs to implement improved models and workflows for biogeochemical reactions.

The Watershed Function SFA seeks to determine how perturbations to mountainous watersheds impact the downstream delivery of water, nutrients, carbon, and metals. The vast study area of the East River Watershed, a representative mountainous watershed in the Upper Colorado River Basin, contains pronounced gradients in hydrology, geomorphology, or type of biome. This represents a challenge for models, especially for the aggregation of the system behavior across subsystems and scales. In this partnership, we are developing the software tools and workflows required to enable a multiscale framework that relies on multiple resolution unstructured meshes to dynamically adjust the process resolution and efficiently perform the simulation over large spatial extents. Development is primarily based on the ATS with a specific emphasis in the newly available reactive transport capabilities. A critical aspect of the work is on the meshing tools (e.g. LaGriT, pylagrit) that support the generation of unstructured meshes with variable resolutions. Development of reaction networks to describe biogeochemical transformations is a central component of the SBR research. All SFAs in one form or another develop and use reaction models for aqueous complexation, surface complexation, mineral dissolution-precipitation, and microbially mediated reactions. In particular, the SLAC, LLNL and ANL SFAs focus on developing mechanistic models of biogeochemical transformations in subsurface environments at fine scales, using molecular, genomic, metabolic, solid-phase, and aqueous chemistry data. Collaboration with IDEAS-Watersheds focuses on two major aspects: (1) developing new approaches and workflows to incorporate new data and knowledge into the reaction models, including the derivation of reaction networks from metagenomics data and reaction parameters; and (2) implementing reaction models that reflect the new understanding in existing codes.

Poster #22-12

IDEAS-Watersheds Continental Modeling Platform and Simulations

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Continental hydrology is one of three cornerstones of the IDEAS-watersheds project. Our goal is to develop a high resolution, integrated hydrologic modeling platform for the Continental US (CONUS) that bridges across the IDEAS-watersheds study areas and provides a scaling framework from the reach to the watershed and the continent. This framework provides unique capabilities to generate multiscale workflows and address outstanding questions regarding large scale groundwater surface water interactions. An initial CONUS model spanning the majority of the continental US was developed using ParFlow-CLM in the first phase of the IDEAS project. Moving forward, the proposed continental modeling will build from the existing CONUS model, applying a phased approach over the next three years to explore multiscale, multi-physics treatments of terrestrial hydrology modeling from the bedrock into the atmosphere. The CONUS research falls under three categories: (1) model development, (2) software development and sustainability, and (3) continental simulations.

This year *model development* is focused on the expansion of the initial CONUS domain to the entire contributing area of the US. The new domain is designed to align with the National Water Model, incorporating coastlines and improving the treatment of internally draining basins. We are developing improved subsurface parameterizations for the new model, increasing the vertical depth and including better representations of alluvial systems and geologic layering.

Our *software development* efforts are focused on building shared infrastructure and tools to improve simulation efficiency and create reproducible workflows. This includes new tools for model compilation available through GitHub and Docker and new metadata and workflow tracking for simulations implemented with Kepler workflows. Additionally, we have developed the EcoSLIM particle tracking code which provides new capabilities to track particles through the land surface component of the system, in addition to the existing groundwater particle tracking capabilities. EcoSLIM is a critical component of our shared software ecosystem which can be implemented across spatial scales relevant to the broader IDEAS-watersheds team.

Continental simulations with the original CONUS domain are also ongoing. We completed a series of warming simulations to explore connections between groundwater storage and watershed response to increased temperatures. Our results provide the first, large scale evaluation of warming impacts within a modeling platform that directly captures lateral groundwater flow. We show that storage changes in shallow groundwater systems can support increased evapotranspiration with warming thus mitigating plant water stress.

Subsurface Biogeochemical Research

University Awards

Poster #21-18

Forest Stress in the Rocky Mountains During the Last Interglacial Warm Period

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Project: University Award

Growing season temperature is a key determinant of forest stress in the Western United States, which portends reductions in growth, including the possibility of regional forest die-off, as temperatures continue to rise. Here, we look at the ecohydrological effects of warming on Western US forests using interglacial-aged subfossil conifer wood samples from Colorado, USA. New downscaled climate model simulations for this period show canopy warming of ~2-4 degrees and an earlier retreat of snowpack, yet our analyses of the carbon isotopes and tree growth show little evidence of enhanced stress levels relative to today. Results from the oxygen isotope ratios in the sub-fossil cellulose show that an increased utilization of summer rain by the trees compensated for the detrimental forcing associated with higher temperatures. The study shows that changes in summer rain, which are notoriously difficult to model, can alter the trajectory of western US forests even in regions that fall outside of traditional monsoon regimes. A detailed analysis of root water uptake dynamics of conifers will be undertaken in the East River Watershed during the 2019 growing season using a new network of sap flow sensors and water isotope analysis.

Poster #21-56

The Influence of Microbial Priming Effects on the Hydro-bio-geochemistry in the Columbia River and its Tributary Confluences

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Project: University Award

A positive priming effect occurs when the microbial oxidation of terrestrial dissolved organic matter (TDOM) is enhanced by the addition of algal dissolved organic matter (ADOM). However, the prevalence of priming within river-tributary confluences, with often contrasting OM sources and composition, remains unknown. Here, we measure total dissolved organic carbon, dissolved nitrogen, chromophoric dissolved organic matter, dissolved lignin phenols, dissolved hydrolysable amino acids, and the molecular composition of DOM via FT-ICR-MS in the mainstem of the Columbia River and three of its tributaries (Snake River, Yakuma River, and Walla Walla) along an extreme hydrologic east-west gradient in the Columbia River drainage basin. Field replicates and mixtures representing river-tributary confluences were incubated in the dark for 15 days to investigate the response of the microbial community to varying DOM quantity and composition. The Columbia, Snake River, and Yakuma Rivers did not differ in DOC, fDOM, and chlorophyll-a concentrations. However, Walla Walla tributary had significantly greater DOC, fDOM, and chlorophyll-a concentrations, indicative of greater contributions from ADOM than the Columbia River and these other tributaries. The FT-ICR-MS spectra for Walla Walla had significantly more peaks corresponding to amino sugars, carbohydrates and proteins while the Columbia River had more peaks for lignin, unsaturated hydrocarbons, and condensed aromatics. When incubated for 15 days in the dark, the DOC did not decrease for Walla Walla or any of the other river and tributary samples. The DOC did decrease, however, in a mix representing the confluence of the Columbia and Walla Walla rivers, suggesting the microbial consortia of the Columbia River were primed by the Walla Walla DOM. The DOM composition, measured by the number of peaks detected via FT-ICR-MS, were significantly different for several compound classes (lignin, protein, tannin, etc.) in the incubations of unmixed river and tributary samples. However, the primed microbial community in the Walla Walla-Columbia mixture appeared to be indiscriminate of the molecular structure of the DOM as the peak count for each compound class did not change significantly. This provides preliminary evidence that the enzymes exuded during aquatic priming can hydrolyze diverse OM structures. Overall, our results indicate the presence of microbial priming effects generated by confluences that mix contrasting OM quality.

Poster #21-61

Methane and Nitrous Oxide Pore-Water Concentration and Flux at the Hyporheic Zone of a Large River

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Project: University Award

Greenhouse gas (GHG) emissions from rivers are a critical missing component of current global GHG models. Their exclusion is mainly due to a lack of in-situ measurements and to a poor understanding of the spatiotemporal dynamics of GHG production and emissions which prevents optimal model parametrization. In this project, we are conducting data-driven field research on the hyporheic zone of a river shore section of the Columbia River. We aim to understand at an ecosite scale: (i) where and when are GHGs produced and if the production is impacted by river stage, (ii) what microbial processes control production and consumption of GHGs and, (iii) what is the effect of environmental conditions on GHG production at the Columbia River nearshore environment and what is the scale in which they operate and could be best modeled. We are using a multidisciplinary approach combining pore dialysis peepers to determine pore water concentration of GHGs, co-located GHG flux measurements with non-steady-state accumulation chambers, meta-omics of microbial communities in the sediment profile to identify microbial processes, and modeling to scale and interpret the observations. We have installed nine peepers in three transects covering shallow, intermediate and deep-water levels. Measurements of pore water concentration of methane (CH₄) and nitrous oxide (N₂O), and co-located flux measurements, were conducted during three different hydrological conditions (rising, falling and falling highly-regulated river stages). Overall, integrated CH₄ porewater concentrations along the sediment profile followed a pattern similar to that of CH₄ fluxes for the three water levels of the gradient during the hydrological conditions considered. However, hotspots in porewater concentrations occurred at different depths in the profile, indicating the influence of groundwater mixing in the patterns observed. In turn, N₂O porewater did not show discernible patterns for the hydrological conditions, and fluxes did not show statistical differences along the gradient of water levels. The next steps in our study are to link concentration and flux results with metagenomic and metatranscriptomic data to help explain the patterns observed (or lack thereof), and parametrize the biogeochemical model *ecosys* to represent individual microbial processes and evaluate their scaling across depths and spatially distinct sites. We expect that our findings help improve predictive understanding of how watersheds function as complex hydrobiogeochemical systems. We also envision that data and results generated in this project will benefit reactive transport models of microbial carbon cycling that can be integrated into the U.S. DOE ACME Land Model (ALM).

Poster #21-62

Respiration in Hyporheic Zones: Advancing the Understanding of Coupled Transport and Microbial Biogeochemistry and their Representation in Open-source Mechanistic Models

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Project: University Award

Hyporheic zones (HZs) are a key feature of river corridors because of substantial carbon and nutrients processing which happen in them. This processing is a cascade of microbially-mediated reactions. The most important of these reactions is respiration since it is thermodynamically favorable and the consumption of oxygen during respiration sets up a cascading redox ladder.

This project's goal is to improve the understanding of respiration in HZs. We seek predictive capabilities that can represent HZ processes in system-scale models. The project is broadly divided into the intertwined tasks of advancing mechanistic models and the mapping and monitoring of reactions and the microbial communities responsible for these in real-scale laboratory flume experiments. The flume experiments use real river water and have been continuously running for months. Direct measurements of CO₂ production and O₂ consumption in both the overlying channel water and throughout the HZ sediment reveal that there is substantial respiration and that the rates vary with HZ depth. The distribution of respiration-sensitive reactive tracers independently support the occurrence of respiration. Microbial community characterization shows that the communities in the flume are similar to those in natural river settings. The communities occupying oxic and anoxic zones are distinct. The experiments show that the CO₂ in the channel, which presumably is evaded to the atmosphere, is largely produced in the sediment and delivered to the channel by hyporheic return flow. This finding emphasizes the importance of considering the HZ, the channel and the overlying atmosphere as one continuum with fully, two-way coupled components. Thus, we are also advancing the modeling of processes that transcend the sediment-water-air interfaces. The model we have developed is called *hyporheicFoam* which is based on the open-source model OpenFOAM. It solves the Reynolds Averaged Navier-Stokes and modified Richards equations for the turbulent open-channel flow and flow in the porous sediment respectively. It takes user-specified biogeochemical reaction networks. Just as we observed in the flume experiments, modeling with *hyporheicFoam* showed that CO₂ produced from respiration in the HZ is released to the channel and eventually to the atmosphere. Our observational and modeling study is the first to show these facets of HZ respiration. Future plans include experimental and modeling assessment of the many factors which control HZ respiration including different forms and sources of carbon and varying hydraulic conditions. The results of this sensitivity analysis will be synthesized into quantitative predictive models.

Poster #22-30

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

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Project: University Award

Aquatic ecosystems display strong coupling between hydrologic conditions and the cycling of carbon, nitrogen, and other major elements as well as trace metal micronutrients and contaminants. In many such systems, sharp redox gradients can produce spatially-varying regions of biogeochemical activity. The biogeochemistry of subsurface zones of aquatic systems has been widely explored from the perspective of redox conditions, substrate availability, and thermodynamic controls on metabolic processes. However, an additional yet under-examined constraint is the availability of trace metal micronutrients. An array of metalloenzymes are essential to many biological pathways associated with microbial carbon and nitrogen cycling and mercury methylation. Laboratory studies using isolate microorganisms have demonstrated that low metal availability inhibits key biological pathways, but similar limitations in natural and human-impacted systems have not been widely investigated. The project thus seeks to establish whether aquatic systems display trace metal limitations on biogeochemical carbon, nitrogen, and mercury transformations. We hypothesize that solid-phase speciation is the primary control on metal availability and that biogeochemical processes utilizing a pathway containing a single, metal-bearing enzyme are most susceptible to metal limitations. This project integrates field and laboratory studies of trace metal availability and biogeochemical processes occurring in wetland soils and hyporheic zone sediments. Our primary field sites include a riparian wetland in the Tims Branch watershed at the Savannah River Site and marsh wetlands at Argonne National Laboratory, both in collaboration with the Argonne Wetland Hydrobiogeochemistry SFA, as well as the hyporheic zone of East Fork Poplar Creek (EFPC) at Oak Ridge National Laboratory in collaboration with the ORNL Mercury SFA. These studies are supplemented by work in marsh wetlands at Marais Temps Clair Conservation Area near St. Louis, MO. In the first half- year of this project, our efforts have focused on key initial tasks. Preliminary measurements showed that the addition of nickel to incubations of marsh soil increased methane production by a factor of 10. We have pursued similar studies using stream sediments from EFPC to explore whether cobalt addition affects mercury methylation. No clear trend was observed, but future work will examine longer incubation times. Soil, sediment, and water sampling at both the EFPC and marsh wetlands at Argonne have investigated the controls on trace metal availability. Planned sampling at the Tims Branch riparian wetland along with incubation experiments using materials from all field sites will further assess the impact of trace metal availability on biogeochemical cycling.

Poster #21-17

Quantifying Subsurface Biogeochemical Variability in a High Altitude Watershed During Winter Isolation

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Project: University Award

Subsurface ecosystems in high-altitude watersheds are influenced by hydrologic events that drive the availability of compounds for biotic and abiotic chemistry. Much of this biogeochemistry occurs in the dynamic hyporheic zone (the interface of the river sediment and groundwater) and in groundwater. Hyporheic systems are conspicuously responsive to hydrologic events, and therefore have the ability to alter surface ecosystem geochemistry. High-altitude systems experience isolation during the wintertime due to unsafe or inclement conditions that prevent access to the watershed for research, and consequently many of these systems are not sampled during the winter months. This isolation leads to a distinct gap in biogeochemical knowledge of these systems, which ultimately affects the accuracy and confidence in which these systems are computationally modeled. We deployed and subsequently retrieved OsmoSamplers from the East River (ER), CO watershed to study the aqueous and gaseous chemistry of the waters from the aquifer, river, and hyporheic zone during the winter. Our Shumway well sampler detected ca. 10x higher concentrations in Cl^- at the end of winter than during the rest of the year, adding to data previously collected only when the well could be accessed. The sampler also validated sustained low levels of SO_4^{2-} in groundwater through late fall and winter months showing an upward trend as summer started. Methane in the well was near saturating levels through the year. Our 10-month sampler installments in the ER surface water revealed up to 50 μM levels of methane in July through September, an increase compared to ca. 5 μM during most months. In contrast, samples from 20-cm deep in the hyporheic zone showed a spring-to-early summer peak in methane (< 65 μM) before declining. A second set of OsmoSamplers is being used to study the microbiome and metatranscriptome of the ER system. These measurements aim to accurately capture the biogeochemistry of the dynamic hyporheic ecosystem's response to hydrologic seasonality in high-altitude watersheds, strengthening our understanding of these systems during the winter months.

Poster #21-63

Persistent Effects of Forest Harvest on Dissolved Organic Matter Composition in Subsurface Hillslope Runoff

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Project: University Award

Timber harvesting commonly alters soil nitrogen (N) and carbon (C) inventory and associated biogeochemical processes the initial years after treatment, yet changes in critical zone processes as forests recover from harvesting remain poorly understood. In high-elevation conifer forests of the Rocky Mountains, slow tree growth and short growing season prolong post-harvest ecosystem responses. Here we analyze hillslope-scale subsurface flow at the Fraser Experimental Forest to evaluate differences in nutrient export and dissolved organic matter (DOM) composition between old-growth and second-growth forest more than three decades after clear cut harvesting. Runoff passing through the upper 3 m of the soil profile was collected before, during, and after peak subsurface discharge during 2017 and 2018. In the second-growth stand, runoff nitrate concentrations were significantly higher and dissolved organic C concentrations were lower relative to the old-growth forest. Dissolved organic N was an order of magnitude higher than dissolved inorganic N concentrations in both forest conditions. Fluorescence spectroscopy of subsurface flow showed contrasting DOM composition from the old- and second-growth forests. The old-growth forest was composed of more complex, aromatic DOM and microbial-like DOM was more prevalent in the second-growth forest. Subsurface flow C:N ratios were twice as high in the old-growth forest and correlated with DOM characterization indices based on fluorescence spectroscopy. Further, biological oxygen demand assays showed that DOM exported from the second-growth forest was consumed 50% more rapidly than that from the old-growth forest. Old-growth and second-growth forests are common within managed landscapes and this hillslope scale comparison will advance understanding of long-term changes in critical zone processes that regulate watershed C and N export and downstream water quality.

Poster #21-15

Snow Accumulation and Melt Simulations in Dry Through Wet Years in the East River

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Project: University Award

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 are implementing a physically-based snow cover evolution model (SnowModel; Liston et al., 2006) at multiple grid resolutions, using different combinations of accumulation process sub-models, over a recent set of years spanning high and low peak accumulation values. These simulations, forced with high-resolution mesoscale model (WRF) output, are compared with ground measurements as well as snow depth and snow water equivalent (SWE) maps from Airborne Snow Observatory flights. These initial results help characterize the snow hydrologic system in the East River, and set the stage for future snow data assimilation work and for integration with simulations of connected systems within the SFA.

Reference:

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

Poster #22-36

Use of Stable Mercury Isotopes to Assess Mercury and Methylmercury Transformation and Transport across Critical Interfaces from the Molecular to the Watershed Scale

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Project: University Award

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 the Hg associated with streambed sediments, streambanks, and floodplain soils resides in relatively insoluble fractions, and has thus been considered to have little impact on dissolved total Hg (THg) concentrations. However, recent studies comparing hydrologic discharge and THg flux from Y12 and Lower EFPC suggest that additional dissolved Hg from the hyporheic pore water or groundwater discharge may variably contribute as much as a third of downstream dissolved Hg loads during baseflow conditions. Thus, the over-arching goal of this project is to use natural Hg stable isotope signatures, imparted by molecular-scale reactions, to gain a more comprehensive quantitative and mechanistic understanding of the processes that supply dissolved Hg to surface water, drive observations of watershed-scale Hg fluxes, and result in the bioaccumulation of methylmercury (MeHg).

To achieve this goal, we are combining an intensive multi-seasonal field study with mechanistic laboratory experiments. First, we are coupling the Hg isotopic composition of dissolved Hg in stream water and in critical subsurface ecosystem compartments (i.e., hyporheic zone, riparian floodplains, and groundwater) with hydrologic flux measurements in four gauged reaches of EFPC. This will enable us to establish an isotope mass balance that assesses the relative importance of dissolved Hg contributed to the stream across these critical interfaces.

Second, we are utilizing sequential extraction methods to characterize the isotopic composition of legacy Hg potentially re-mobilized from streambed sediment. This will provide insight into the sources and mechanisms that replenish the supply of dissolved Hg within critical subsurface zones. Third, we are assessing the isotopic composition of MeHg in biota of EFPC, as a step toward identifying the source(s) of bioaccumulative MeHg in the EFPC ecosystem.

Here, we present: (1) Hg concentration and isotopic composition of all surface water, hyporheic pore water, and riparian groundwater samples analyzed to date; (2) isotopic mass balance assessments regarding legacy inputs of dissolved Hg to the stream water of EFPC; (3) sequential extraction results showing potential re-mobilization of recalcitrant legacy Hg from streambed sediment; and (4) measurements of the isotopic composition of MeHg accumulating in biota of EFPC.

Poster #21-16

A Radioisotope-Enabled Reactive Transport Model for Deep Vadose Zone Carbon

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In upland forested hillslopes, such as those observed across the East River watershed, roots extend well beneath the classically defined soil layer into partially weathered, unsaturated rock to access both water and nutrients. Yet current carbon cycle models rarely extend below shallow soils, and the contribution of this deeper subsurface nutrient cycling to carbon stocks and fluxes is virtually unknown. We are now directly constraining this previously disguised component of the carbon cycle through a novel Vadose zone Monitoring System (VMS) installed at the Eel River watershed in Northern California, which is similarly underlain by a shale lithology and hosts a mature forest ecosystem. The VMS consists of a pair of sub-horizontal bore holes instrumented with flexible plastic sleeves which allow both passive and active suction cup sampling of fluids draining through the partially saturated shale weathering profile, as well as gas sampling ports, moisture and temperature sensors. Our exploratory efforts are now constraining carbon stocks and fluxes as an analog to the hillslopes of the East River, providing new evidence that approximately 30% of net CO₂ flux from the terrestrial environment to the atmosphere is sourced many meters below the soil layer. We have shown that this CO₂, though produced well below what would classically be defined as soil, is radiocarbon modern. Thus, in total, this work indicates that modern carbon is being delivered rapidly to the deep subsurface, likely as a result of the rooting depth of mature trees, and this previously undocumented carbon cycle is a substantial component of the CO₂ generated in the terrestrial environment. To extend these results, we are now working with the LBNL SFA team to generate comparable datasets of CO₂ and O₂ gradients, complementary fluid phase DIC and DOC, and radiocarbon to constrain the contribution of deeply rooted vegetation to this subsurface carbon cycle. Modeling will be supported by the radioisotope-enabled version of CrunchTope, capable of simultaneous and explicit simulation of the three isotopes of carbon including both stable isotope fractionation and radioactive decay. Model development has been completed and aspects have been benchmarked against several other multi-component software platforms. Through this advanced modeling capability, the rates of carbon oxidation, contribution to weathering and thus the development of soils and sustainability of forest ecosystems will be embedded within an adaptive and predictive model framework.

Metabolic Constraints of Organic Matter Mineralization and Metal Cycling During Flood Plain Evolution

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Floodplains are poorly understood and dynamic components of the global carbon cycle that are not well represented in Earth system models. Further, they have a dominant influence on the cycling of important metals within critical transport conduits between surface waters and groundwater. The physical characteristics of floodplains make the hydrology and associated coupled biology and geochemistry particularly responsive to ongoing and impending changes in climate, river management, and land development.

Using a combination of field-scale measurement with micro-scale laboratory experiments, we find that oxygen diffusion limitations lead to heterogeneous redox profiles, shifting microbial metabolism to less efficient anaerobic SOC oxidation pathways. During flooded periods, exhibiting strongly reducing conditions, DOC concentrations are elevated yet microbial C oxidation is limited by thermodynamic constraints on anaerobic respiration. Through laboratory incubations, we observed both kinetic and thermodynamic controls on carbon oxidation; anaerobic incubations were tested with nitrate and sulfate addition relative to an anoxic control and compared against aerobic conditions. Under anaerobic conditions, oxidation rates are consistent with thermodynamic succession in energy yields. Carbon oxidation rates are, however, highly sensitive to oxygenation, particularly in previously anaerobic soils, where oxidation rates are maximized. However, under field conditions, after a short-lived rise in C oxidation, rates decline again due to the formation of metal-organic complexes, which restrict the availability of DOC for microbial respiration. Our results suggest that these seasonally shifting controls on C oxidation rates across the floodplain are critical controls on C and metal export from the floodplain.

Export of metal-organic complexes varies depending on the hydrologic condition of the floodplain. We observe different metal-organic complexes, and the preference for metals of differing chemistry, depending on the metabolic conditions of the soil. Combining our biogeochemical measurements with hydrological investigations of the East River flood plain, we are developing a reactive transport modeling framework that examines carbon and metal transformations and export to river water. A multi-level well-field providing the capacity for determination of hydrologic gradients and pore-water chemistry is being utilized within two contrasting river meanders, representing end-members of hydrologic conductivity and oxygenation. Collectively, our results illustrate the combined, and dynamic, impacts of mineral- associations and metabolic controls on carbon and metal fate. The highly variable hydrology of floodplains leads to concomitant changes in biogeochemical processes within soils that ultimately control organic carbon, nutrients, and metal cycles.

Poster #22-18

Molecular and Genomic Insights into Nitrogen-Cycling Microbial Communities within the Terrestrial Subsurface at Riverton, WY

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Floodplains are hot spots for biological productivity that drive biogeochemical reactions and moderate ground and surface water quality, carbon turnover, and regional land-atmosphere interactions. Within the semi-arid upper Colorado River Basin (CRB) and intermountain west, a large fraction of shallow subsurface organic carbon (C) is believed to reside within fine-grained, organic-enriched sediments known as naturally-reduced zones (NRZs). NRZs, formed within the numerous contaminated DOE legacy site floodplains in the upper CRB, contain large inventories of nitrogen (N) and uranium (U). Microbial N-cycling has the capability to “unlock” the biogeochemical nutrient supply stored within NRZs, drive C cycling, and liberate U to the aquifers. Nitrification links organic matter decomposition to the production of nitrite and ultimately nitrate, an oxidant of U(IV) and the primary electron acceptor for denitrification. Nitrification and denitrification help mediate C turnover in NRZ sediments and are also the primary sources of the potent greenhouse gas, N₂O. Despite their biogeochemical importance, remarkably little is currently known regarding N-cycling microbial communities within terrestrial subsurface soils/sediments, let alone NRZs.

To address this critical knowledge gap, we are examining N-cycling communities at the DOE legacy U ore processing site in Riverton, WY, using a combination of molecular, meta-omic, biogeochemical, and modeling approaches. In addition to documenting the distribution and diversity of ammonia-oxidizing *Thaumarchaeota* using functional gene and high-throughput 16S rRNA amplicon analyses, we have recently obtained metagenome-assembled genomes (MAGs) from these biogeochemically-important *Archaea* from multiple depths within the Riverton subsurface. Ultimately, this multi-pronged approach will yield valuable genomic, ecophysiological, and biogeochemical insights into key microbial N-cycling guilds within the terrestrial subsurface.

Poster #21-11

On Dry Season Transpiration

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Water is the principal regulator in biosphere-atmosphere interactions. High-frequency observations at a steep hillslope in the Mediterranean climate of northern California show that different proximate evergreen species have very different transpiration seasonality. A surprise is that Pacific Madrones show maximal daily transpiration in the dry summer season, with concomitant impacts on local energy and CO₂ exchange (Link et al. 2014). We hypothesize that the tree roots at the site have access to a deep store of water, as the water table some 20 meters below the surface exhibits very dynamic fluctuations with every rain storm. With DOE support, we have developed a stochastic parameterization of hydraulic conductivity that takes into account preferential flow through weathered bedrock (Vrettas and Fung, 2015), and applied the Richards Equation with the new parameterization to investigate the impact of subsurface water storage capacity (especially in the weathered bedrock) and rooting structure on the timing and magnitude of transpiration (Vrettas and Fung, 2017). The results show that it is the root mass below 4 meters that access the moisture in the weathered bedrock.

We have analyzed USDA Forestry Inventory and Analysis DataBase (FIADB) and mapped the spatial distribution of the 98 tree species in California. Our analysis shows tree mortality during the 2012-2016 drought does not map onto precipitation deficits for the period, but corresponds with differences in the root structure of the different species. We thus hypothesize that deep water stores accessible to deep roots are not unique to the research site, and could explain differential resilience to droughts and insect infestations across a landscape.

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Poster #21-74

Physical, Resource Supply, and Biological Controls on Nutrient Processing Along the River Continuum

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Excess nutrient loading has negatively impacted the ecology of ~90% of the streams in the US and the ecosystem services these streams provide, with estimated damages to US surface and groundwater system over of 100 billion dollar per year. Thus, there is a strong need to develop methods to predict the transport, uptake, and export of nutrients along fluvial networks and their cumulative effects on surface and groundwater quality. Our project is developing a data-driven, mechanistic understanding of critical factors that largely control nutrient uptake and export: 1) interactions between transport-related processes (mass- transfer to metabolically active zones), 2) resource supply dynamics (nutrient concentrations, stoichiometric constraints, etc.), and 3) biological controls (microbial community structure and function), and how these key factors drive nutrient uptake along a river continuum. This work is designed to address current knowledge gaps in understanding lotic nutrient dynamics that include a paucity of data for high order streams, a lack of studies assessing stoichiometric controls on nutrient uptake due to a traditional focus on solute-specific analyses (e.g., nitrogen only), and a scarcity of data that links microbial diversity and function with nutrient uptake dynamics along fluvial networks. Resolving these limitations will promote scientifically based restoration projects to reduce the burden of eutrophication costs. To meet our goals, we are pursuing three specific research objectives: RO1) Investigate how changes in river sediment texture control mass-transfer to metabolically active zones, colonizable surface area, and biological nutrient uptake along the river continuum; RO2) Investigate nutrient uptake kinetics along the river continuum considering limiting vs. non-limiting (i.e., stoichiometrically balanced) conditions, and labile vs. recalcitrant organic matter sources; and RO3) Investigate differences in microbial diversity, community structure, and genomic potential along the river continuum and how differences interact with resource supply to impose fundamental controls on nutrient uptake.

We are performing our research in a river continuum that spans four orders of magnitude in mean annual discharge (10^0 – 10^3 L/s), more than 2000 m in altitude, and more than 500 km of stream longitude. We incubated novel hollow-core columns filled with native and standardized sediments at each of the eight stream orders along the continuum for three months. The columns will be transported to the lab where tracer experiments will be performed under standardized flow conditions. Conducting the experiments with the two sediment types will provide the information necessary to determine how transport, normalized (by colonization and surface area) nutrient uptake rates, and variation in the biological community interact to influence nutrient uptake along the river continuum. Additionally, two resource supply injections will be performed on each of the columns: an only nitrate addition, followed by a stoichiometrically 'balanced' 106C:16N:1P addition. The stoichiometrically balanced injections will provide information necessary to determine how limitations for a given resource may impact nutrient uptake scaling in streams.

Our research seeks to depart from the status quo of focusing on solute-specific, site-specific nutrient uptake analyses, which have resulted in unscalable frameworks, to incorporate a more holistic, stoichiometrically and microbially based, data-driven mechanistic understanding of nutrient uptake and export along fluvial networks.

Poster #21-65

Water Management Impacts on Groundwater-River Water Exchanges

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Human activity along river corridors disturbs many critical river processes, including surface- groundwater exchanges. In many rivers, these exchanges provide important exchanges of energy, biota, and solutes between the surface and subsurface environments, and support fisheries and removal of some pollutants from rivers. This project aims to determine if water management activities within and beyond the river corridor impact groundwater exchanges. To determine this, we are studying the Hanford Reach of the Columbia River, in Southeast Washington. Since there are many challenges to using applied tracers in a large river system, this project aims to use natural tracers to determine locations of groundwater inflows, by taking water quality and GPS measurements along the streambed during boat surveys throughout the year. These measurements indicate the presence of groundwater inflows at the riverbed at several locations. We compare these inflows against locations of irrigation return flow and lateral contributing area to the exchange to identify the influence of each on river-groundwater exchange.

Several of these inflows show higher than main-channel levels of nitrate, suggesting impact from nearby shoreline irrigation. These insights will improve calibration models of hydrologic exchange developed by the River Corridor SFA at the reach scale of the Columbia River, as well as advance knowledge about the connection of landscape management to large river systems.

Poster #21-66

M&M: A Multi-Fidelity & Machine-Learning Approach to Model Hydrologic-Biogeochemical Processes in the Groundwater-Surface Water Interaction Zone

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We have developed a *multi-fidelity deep learning approach* suitable for optimal data acquisition, model discovery, model parameterization, and, ultimately, for predictive modeling of geo-physico-chemical processes for the Hanford site. Using a one-year exploratory grant we have developed a new multi-fidelity capability that has a tremendous potential for modeling hydrologic- biogeochemical processes in the groundwater-surface water interaction zone. We presented these results to SFA leader Dr. T. Scheibe and his team (January 23, 2019). We started with Gaussian Process Regression but we switched to deep neural networks (DNN) for easier training and scalability. We have designed a new architecture of a multi-fidelity physics-informed neural network (PINN) and obtained some results for solving the equation for unsaturated flows for the pressure height h . We assumed that we have *only two experimental measurements* and that we have several points from the FPLOTRAN simulation, which may not be very accurate. By using the multi-fidelity PINN we are able to obtain the correct solution and discover the correct hydraulic conductivity.

Poster #21-4

Root Influences on Mobilization and Export of Mineral-bound Soil Organic Matter

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Biogeochemical cycles within mountainous watersheds are key regulators of ecosystem carbon storage and downstream nutrient loadings, and they have shown to be particularly vulnerable to climate change impacts. Increasing temperature and persistent droughts have already dramatically changed vegetation cover across the mountainous western US, with unknown consequences for carbon and nutrient cycles in soils belowground. What remains elusive is to what extent associated changes in root-soil interactions may mobilize the vast pool of organic matter (OM) that has been stabilized by associations with minerals for centuries or millennia. Although plant root-driven OM mobilization from minerals may be a central control on carbon loss and nutrient export, such mechanisms are currently missing from conceptual and numerical models.

The overall goal of this project is to identify the (bio)geochemical mechanisms by which roots destabilize mineral-OM associations and the cumulative impact of OM mobilization on the fate of carbon and nitrogen. To accomplish this goal, we initiated model system experiments to assess the vulnerability of isotopically labeled OM bound to different soil minerals to various root-driven mobilization strategies. Our results show that OM bound to mineral phases with the greatest sorptive capacity are also the most susceptible to root-driven mobilization. We further highlight ongoing greenhouse experiments, as well as field-based experiments aiming to quantify the impact of root-driven OM mobilization across a hillslope transect in the subalpine East River watershed.

In addition, we have developed a well-controlled “rhizobox” approach to identify the (bio)geochemical mechanisms roots employ to mobilize OM from minerals. Using a combination of spatially-resolved micro(bio)sensors and high-resolution mass spectrometry, our results show how growing roots of *Festuca thurberi*, an abundant grass species across the East River watershed, alter the composition and availability of OM on extremely short time scale. Our data show that OM mobilization in the rhizosphere is linked to root growth, which promotes diurnal changes in redox and pH that control metal precipitation/dissolution. By parameterizing a rhizosphere (hydro)biogeochemistry reactive transport model, we are able to show that such OM dynamics in the rhizosphere are directly related to rhizodeposition and water fluxes. In sum, our initial results validate the strong control plant roots exert on the stability of mineral-OM associations in the rhizosphere and, thus, on the potential for C and N export from watersheds.

Poster #21-5

Distinct Source Water Chemistry Shapes Contrasting Concentration – Discharge Patterns

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Project: University Award

Contrasting concentration-discharge (C-Q) behaviors have been observed for the same solute in different watersheds and for different solutes in the same watershed. A unified mechanistic understanding however remains elusive. This work tests the hypothesis that seemingly disparate C-Q behaviors are driven by switching dominance of end-members contributing to streams and their concentration contrasts arising from subsurface spatial heterogeneity. We use data from Coal Creek, a high-elevation mountainous catchment in Colorado and a recently-developed watershed reactive transport model (BioRT-Flux-PIHM) to gain mechanistic understanding; Monte-Carlo simulation (500 cases) casts the results under broader conditions. Results show that the switching dominance in the stream between organic-rich soil water during spring melt and organic-poor groundwater under dry conditions leads to flushing patterns of dissolved organic carbon (DOC). Dilution occurs for geogenic species (e.g., Na, Ca, Mg) that are abundant in groundwater with reactive rocks at depth. Monte-Carlo simulations indicate that concentration differences between soil and groundwater as end members determine the slopes (b) of C-Q patterns with a general relationship

$$b = (\delta_b C_{ratio}) / (C_{ratio,1/2} + C_{ratio}) + b_{min}$$

At low ratios of soil water versus groundwater concentrations ($C_{ratio} = C_{sw} / C_{gw} < 0.6$), dilution occurs; at high ratios ($C_{ratio} > 1.8$), flushing occurs; chemostasis occurs in between. The b values of 11 solutes (DOC, dissolved phosphorus, NO_3^- , K, Si, Ca, Mg, Na, Al, Mn, Fe) from three watersheds (Coal Creek, Shale Hills, Plynlimon) follow this equation. This indicates potentially broad applications of this equation to quantify b values given end-member concentrations in watersheds of diverse climate, geology, and land cover conditions.

Poster #21-6

Regolith, Rock and Fluid Distributions at the Upper Colorado River Basin via a Multicomponent Seismic Imaging Approach

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Project: University Award

Surface geophysical measurements can link geologic, geomorphic and hydrologic processes. Characterizing subsurface properties at sufficient resolution, yet over a large enough spatial extent to make statistically relevant correlations between subsurface structure and surface observations (topographic attributes, vegetation, etc.), is currently not standard practice because ground-based geophysical campaigns are limited by acquisition rates. The seismic land streamer is a semi-autonomous vehicle-mounted acquisition system designed to pull geophone arrays and a seismic source to rapidly acquire large data volumes compared to traditional planted geophone surveys. Acquisition geometry is well suited for obtaining first arrivals to constrain p-wave velocities (V_p), Rayleigh waves to constrain shear-wave (V_s) velocities and reflections to map significant subsurface stratigraphy. Joint and/or independent analysis of these semi-independent data sources reduce uncertainties in data interpretation.

In October 2018, we conducted an exploratory seismic survey of the East River Watershed Function Science Focus Area, near Crested Butte, CO. Our survey goals were to map seismic bedrock, regolith and sediment properties and relate them to geomorphic and hydrologic processes. Bedrock in the watershed is composed of Mancos Shale and younger crystalline intrusions. Hillslopes are mantled with weathered bedrock, moraines, landslides and colluvium. The watershed is roughly divided into an upper and lower flood plain separated by a locally steeper stream gradient with bedrock exposures in the river. We acquired ~12 km of seismic data along roads with a 72-channel, 1.25m spaced streamer and an average shot spacing of 2.5m and an average acquisition rate of 3 km/day. We also obtained ~3km of planted geophone data with geophone and shot spacings between 2.5 and 5 meters and an acquisition rate of 0.5 km/day.

Preliminary V_p results show a sharp transition between regolith and bedrock along hillslopes suggesting a similarly abrupt change in porosity. V_p anisotropy in the Mancos Shale suggests geologic structure drives bedrock groundwater flow. We note changes in V_p and V_s with elevation and slope, reflecting contact metamorphism away from intrusive rocks and the influence of sediment transport on seismic velocity. We show that the Upper Flood Plain contains about 20 meters of alluvium compared to <10 meters in the Lower Flood Plain, reflecting slope-dependent variations sediment transport along the watershed. Reflection images suggest channel morphology is controlled, in part by geologic structure.

Poster #21-7

Soil Respiration Across Scales

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Soil respiration fluxes play a fundamental role in the terrestrial carbon cycle. Nevertheless, representing the processes that drive soil respiration in models remains an outstanding challenge due to an array of spatially- and temporally-dependent sensitivities to environmental drivers. In particular, the interactions between these drivers, such as plant phenology, temperature, and soil moisture remain largely uncharacterized. Another outstanding challenge is in partitioning between the heterotrophic and autotrophic components of respiration. To address these challenges, we have conducted incubation studies of soil respiration, characterized soil carbon stocks using spectroscopy and radiocarbon, and measured soil respiration rates in a subalpine meadow within the East River watershed, Gothic, CO over the 2016, 2017, and 2018 growing seasons. Laboratory incubations studies with variable soil moisture were used to test a moisture-dependent model framework for microbial respiration that captures the transition between dormant and active states. When the model is run using field measurements of soil moisture and soil carbon, the model successfully matches deep late season CO₂ profiles. To further constrain the parameters of this modeling framework, we are now extracting RNA/DNA ratios as a function of time to monitor the timescale of transition between active and dormant states. To quantify total soil respiration and understand how microbial processes translate to plot-scale measurements, we quantified depth- resolved net CO₂ production rates using observations of soil pCO₂ and surface efflux rates to drive a 1-D diffusion-reaction model. These rates were then compared to sensor monitoring data of soil moisture and temperature and to the MODIS satellite-derived enhanced vegetation index (EVI) as a proxy of plant phenology. A comparison of MODIS EVI across the field site between years demonstrated that when rain events occurred late in the growing season, as vegetation is senescing, soil respiration is significantly less responsive to increased soil moisture. Future work will examine the extent to which the plant response is further mediating the microbial response, potentially due to a reduction in exudate input. We also observe significant fluxes of CO₂ from the deep subsurface (> 165 cm) in the late growing season that likely persist under snowpack. Collectively, our results suggest that (1) plant phenology regulates the response of soil respiration rates to pulse wetting events and (2) deep subsurface carbon fluxes may constitute a significant portion of integrated annual surface CO₂ fluxes. Both processes will need to be adequately reflected on model representations to fully capture the response of ecosystems to a more variable water cycle.

Poster #21-8

Measuring the Link Between Energy and Water: Latent Heat Flux in Heterogeneous Mountain Environments

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Snowpack in high elevation regions of the Colorado River basin contributes to seventy percent of the Colorado River streamflow, which provides water to thirty million people. Despite the importance of these regions for downstream water delivery, water availability from these mountain sources is vulnerable to the changing climate. However, the effect of climate change on these regions is difficult to characterize given Earth System Models' poor representation of high-elevation, mountainous regions. These regions are difficult to represent in large-scale models due to their large topographic gradients, heterogeneous land cover, and complex atmospheric patterns. Our DOE SBR Exploratory Project has combined observations and models to better characterize water, energy and CO₂ fluxes in a headwaters system. A combination of point observations and high-resolution models are used to estimate these hydrologic fluxes in a Colorado River headwaters region, near Crested Butte, Colorado. Using data from an eddy flux tower collocated with a metrological station in the East River basin, this study has collected almost two years of observations that include latent and sensible heat fluxes. Initial observations are consistent with expected results and within reasonable bounds; latent heat is greatest in the spring as vegetation begins growing and lowest in the winter due to snow cover. Conversely, sensible heat peaks before total snow melt and decreases as latent heat increases. These initial results show promise for accurately modeling energy fluxes and plant water use in this heterogeneous mountain region.

Poster #21-52

Influence of Redox Reactions and Organic Ligand Complexation on Uranium, Neptunium, Technetium Subsurface Transport: Upscaling Laboratory Experiments to Understand Field Lysimeter Data

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The migration of trace elements in the environment is dependent on the chemical species which dominate under given geochemical conditions. The mobility can be enhanced or retarded by altering the oxidation state or forming soluble organic ligand-metal ion complexes. This work examines three case studies to evaluate the impacts of these changes in chemical speciation on the transport of trace elements through soil. Our approach seeks to characterize the time and length scales over which non-equilibrium states are maintained by rate-limiting (or rate-enhancing) reactions between radionuclides and co-reactants due to interactions between physical mass-transfer processes (i.e., flow, advection, diffusion) and (biogeo)chemical reactions.

Neptunium and technetium transport in field lysimeter studies has demonstrated enhanced mobilization of Np and Tc due to oxidation of Np(IV) to Np(V) and Tc(IV) to Tc(VII). Solid NpO₂(s) and Tc amended cementitious waste form samples were deployed in field lysimeters for up to 2 years. The effluent concentrations of Np and Tc were continually monitored and after retrieval from the field, the lysimeters were destructively sampled to determine the solid phase concentrations of Np and Tc as a function of depth in the lysimeter. The retrieved solid phases indicated surficial oxidation of NpO₂(s) along grain boundaries and leaching of Tc from corrosion rinds of the cementitious waste form. Both processes are controlled by redox gradients between the soil pore water and the waste forms. Complimentary laboratory testing has evaluated the rate and extent of source term oxidation and demonstrated that strong reducing gradients downgradient of the source can reduce Tc(VII) to immobile and insoluble Tc(IV). These measurements are enabled by the development of real-time, in-situ radioisotope monitoring techniques by our team.

A second mechanism by which the mobility of ions can be altered is through complexation with organic ligands. This work has examined the influence of nutrient availability, plant roots and plant root exudates on preferential water flow through field lysimeters and dissolution of uranyl phosphate minerals through formation of soluble U(VI)-ligand complexes. Results indicate that less soluble phosphate sources lead to enhanced plant exudate production which in turn enhances uranium solubility and mobility. These results were verified using flow-through batch reactor experiments examining the dissolution of uranyl phosphate by citric acid (a common phytosiderophore). Ongoing field lysimeter experiments with and without plants are examining these processes on larger spatial and temporal scales.

This material is based upon work supported by the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences and Office of Biological and Environmental Research under Award Number DE-SC-00012530.

Poster #21-2

Investigating Bedrock Fractures as a Dynamic Hydrologic Reservoir Across a Gradient in Climate and Erosion Rate

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BER Program: SBR

Project: University Award

The weathered and fractured bedrock that commonly underlies soils in montane environments can be sufficiently porous and permeable to transiently store and transmit water. There is increasing inferential evidence that this variably saturated weathered bedrock region regulates subsurface biogeochemical processes and the partitioning of precipitation between evapotranspiration and runoff. However, observations of hydrologic dynamics in the bedrock unsaturated zone are sparse, and thus the representation of this region in models of land-surface processes remains poorly constrained. This project seeks to evaluate predictions of how the weathering profile is structured at the hillslope scale by assembling direct observations within four sites underlain by clay-rich bedrock (i.e. shale) across a gradient in climate and erosion rates: the Angelo Coast Range Reserve (ACRR), Sagehorn-Russell Ranch (SRR), Antelope Valley Ranch (AVR), and the LBNL Watershed Function Scientific Focus Area (SFA). To complement existing boreholes at ACRR and SRR, we have now established field monitoring sites in forested shale bedrock at the AVR and SFA sites. The boreholes were outfitted with pressure transducers to monitor groundwater levels and we are currently characterizing mineralogy, geochemistry and pore structure on cores.

With the establishment of new boreholes, we have now documented significant water storage in weathered bedrock using low-field borehole nuclear magnetic resonance (NMR) across all four sites. In the upper 4 m of bedrock, the average water contents at ACRR, AVR, SRR, and SFA are approximately 25%, 16%, 25%, 23% respectively. At the ACRR site, where long-term monitoring via neutron probe surveys and time-domain transmission sensors are available, we have demonstrated that NMR reliably records moisture content and importantly, moisture content dynamics in weathered bedrock. Across all sites, our NMR monitoring has also revealed that a considerable fraction of the water storage occurs in fractures or pores that are significantly larger than the fine-grained bedrock matrix of the parent rock. To identify the proportion of water storage occurring in fractures and large pores, we analyzed the NMR signal by evaluating both the sum of echoes and an inversion of the NMR signal for a distribution of T_2 relaxation times. Both methods reveal that at least 20% of the water storage occurs in fractures and larger pores across all sites. To constrain the interpretation of the in-situ field-scale NMR measurements, we are comparing the NMR response of variably saturated core samples to independent pore-structure information obtained via pycnometry and micro-CT. Preliminary results support the inference that dynamic seasonal water storage is dominantly restricted to the fracture network, which can reach 7% of the total volume. This dynamic range in water content is comparable to that of some soils, underscoring the need to understand how this region of the Earth System is structured, and functions as a hydrologic reservoir.

Influence of Hyporheic Exchange on Coupled S-Fe-C Biogeochemical Cycling in Riparian Wetland Sediments

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Project: University Award

Riparian wetland hyporheic zones, where oxic surface water and anoxic groundwater mix, exhibit dynamic conditions that drive steep redox gradients and promote hotspots and hot-moments of diverse and fluctuating microbial activity. There is growing evidence that highly active “cryptic” sulfur cycling processes drive the fate of iron and carbon and respond to dynamic hyporheic fluxes in riparian wetlands. These “hidden” or “cryptic” sulfur redox processes are 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. Our specific objectives are to (1) measure the fate and transport of Fe, S, and CH₄ in dynamic riparian wetlands, (2) evaluate the microbial community structure and potential function driving these cycles, (3) incorporate “cryptic” S-Fe-C processes into a reactive transport model to examine hyporheic flux impacts, and (4) assess how increased sulfate loading can alter coupled S-Fe-C processes. We will present preliminary results of our geochemical analyses (Fe and S speciation and abundance in sediments, porewaters, and surface waters) and hydrologic flux measurements in an organic-rich riparian wetland at Tims Branch, part of the Argonne Wetland Hydrobiogeochemistry SFA. We will compare these results to findings at a riparian wetland site in northern Minnesota with higher surface water sulfate loading, for which we have implemented a reactive transport model that has provided evidence for these cryptic sulfur redox processes.

Poster #21-51

Natural Organic Matter and Microbial Controls on Mobilization/Immobilization of I and Pu in Soils and Waters Affected by Radionuclide Releases in USA and Japan.

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Project: University Award

Examining the short-term deposition and forecasting the long-term fate of plutonium (Pu) is becoming increasingly important as more worldwide military and nuclear-power waste is being generated. Soils from the Fukushima Prefecture provided the opportunity to compare Pu from reactor fallout in the litter layer to that derived from 1960's bomb fallout in the underlying soil. Additionally, we used this unique opportunity to explore the long-term behavior of Pu in Nagasaki sediments, where bomb-derived Pu was deposited in 1945. A combination of selective extractions and molecular characterization via electrospray ionization Fourier-transform ion cyclotron resonance mass spectrometry (ESI-FTICRMS) were used in an attempt to resolve what regulated the long-term stabilization of $^{239,240}\text{Pu}$ in Nagasaki bomb residue-containing sediments (>400 cm) and the short-term deposition of nuclear plant accident-derived $^{239,240}\text{Pu}$ in Fukushima Prefecture (<12 cm). In deep Nagasaki sediments, our results demonstrated that $55\pm 3\%$ of the $^{239,240}\text{Pu}$ was preferentially associated with more persistent organic matter compounds, particularly those natural organic matter (NOM) stabilized by Fe oxides ($\text{NOM}_{\text{Fe-oxide}}$). Other organic matter compounds served as the secondary sink of these bomb-derived $^{239,240}\text{Pu}$ ($31\pm 2\%$ on average), and less than 20% of the bomb-derived $^{239,240}\text{Pu}$ was immobilized by the inorganic mineral particles. In a 9-cm thick, $^{239,240}\text{Pu}$ -enriched layer at ~400cm depth, N-containing carboxyl aliphatic and/or alicyclic molecules (CCAM) in $\text{NOM}_{\text{Fe-oxide}}$ and other NOM fractions immobilized the majority of $^{239,240}\text{Pu}$. Among the cluster of N-containing CCAM moieties, hydroxamate siderophores, the strongest known Pu chelators in nature, were further detected in these "aged" Nagasaki bomb residue-containing sediments. In Fukushima Prefecture and Nagasaki sediments, the NOM still served as the predominant sink for these nuclear plant accident-derived $^{239,240}\text{Pu}$ (sum of $\text{NOM}_{\text{Fe-oxide}}$ and other organic matter). While present long-term disposal and environmental remediation modeling assume that solubility limits and sorption to mineral surfaces control Pu subsurface mobility, our observations suggest that NOM, which is present in essentially all environmental systems, undoubtedly plays an important role in sequestering Pu. Ignoring the role of NOM in controlling Pu fate and transport is not justified in most environmental systems*.

References:

* Lin, P., Xu, C., Kaplan, D.I., Chen, H.M., Sun, L., Yeager, C.M., Xing, W., Sun, L., Schwehr, K.A., Yamazaki, H., Saito-Kokubu, Y., Hatcher, P.G., Santschi, P.H. 2018. Nagasaki sediments reveal that long-term fate of plutonium is controlled by select organic matter moieties. STOTEN, submitted.

Poster #22-3

Constraining Physical Understanding of Aerosol Loading, Biogeochemistry, and Snowmelt Hydrology from Hillslope to Watershed Scale in the East River Scientific Focus Area

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BER Program: SBR

Project: University Award

The mountain snowpack is a critical component of regional hydrology, ecology, biogeochemistry, and climate in the Western US. This project leverages the East River Scientific Focus Area (SFA), as an outdoor laboratory to address a significant gap in our understanding of the mountain snowpack; namely, how atmospheric constituent deposition on snowpack influences snow energy balance and nutrient/chemical cycling, and how snowmelt timing and intensity exerts controls on emergent biogeochemical and ecohydrologic behavior. This aligns with East River SFA goals to integrate landscape scale measurements and physical based modeling tools to improve understanding of controls on runoff production, ecohydrology, biogeochemical cycling, and land surface energy partitioning in high mountain watersheds. We will present current observation and results from the project, including observations of snowpack at multiple scales such as surface elevation and snow reflectance measurements from NASA-JPL's Airborne Snow Observatory, high-resolution measurements of snow and deposited aerosols physical, chemical, and optical properties, and discuss future planned observations for tracking of deposited aerosols residence and reaction times in the watershed, and in situ time series of surface energy balance, water flux, and water chemistry. We will also highlight how we plan to fuse the remotely sensed and ground based measurements with an operational, physics-based hydrologic model, the WRF-Hydro/National Water Model system, to test and improve its capability to represent alpine snow dynamics, and related control on ecohydrologic and biogeochemical processes, from the hillslope to watershed scale.

Multiscale Modeling of Mercury Geochemistry

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Project: University Award

Project Website: <https://aquamer.ornl.gov>

In natural aquatic environments, the transport of mercury (Hg) inorganic and organic complexes takes place in flowing water and simultaneously with equilibrium and kinetic reactions. A web-based multiscale modeling aqueous speciation resource (*AQUA-MER*) has been developed for the aqueous biogeochemical speciation of metals in environment. *AQUA-MER* integrates the calculation of atomistic first-principles based thermodynamic constant with continuum-scale speciation modelling for metals. In general, the continuum-scale speciation calculations use thermodynamic stability constants ($\log K$) to predict the mesoscale distribution of Hg. However, experimental $\log K$ values are not available for many relevant complexes and for others can span ranges in excess of 10 log units. We investigated the effects of $\log K$ uncertainties on speciation calculations. We showed that thermodynamic parameter uncertainties can lead to output concentrations spanning several orders of magnitude and by performing the uncertainty analysis we could identify environmental regimes where uncertainty is important to consider in speciation modeling. Accurate and reliable quantum chemical approaches have been developed and implemented in *AQUA-MER* for the $\log K$ calculation of Hg complexation with inorganic and low-molecular weight organic compounds. High molecular weight dissolved organic matter (DOM) in the natural environment can also bind with Hg, forming stable complexes. However, the experimental $\log K$ values vary between ~ 31 and 42 log units for $\text{Hg}(\text{DOM})_2$ because of the difficulties in the molecular level characterization of the highly heterogeneous DOM. Atomistic MD simulation can capture the details of aggregation and distribution of functional groups in DOM at the molecular level. 100 ns time scale molecular dynamics simulations reveal the initial aggregation of various components of DOM forming complex structures. At the continuum-scale, a travel-time based reactive transport model in the hyporheic zone of stream corridors was established for the multicomponent Hg-DOM-S system and implemented through PFLOTRAN. Sulfur redox zonation was accounted for using a prescribed oxygen gradient. Temporal and spatial distributions of Hg-containing species along the vertical axis of a single sediment bedform were obtained and analyzed. Future studies will focus on integrating the Hg-DOM complexation mechanisms obtained from atomistic MD simulations into continuum-scale reactive transport simulations. We present an information-theoretic approach that allows for seamless integration of multi-resolution data into multi-scale simulations to upscale/downscale hydraulic conductivity of heterogeneous porous formations. Available data (at either the fine- or the coarse-scale) are used to inform models at the opposite scale by setting a probabilistic equivalence between the fine and the coarse scale, with closures (parameters and/or constitutive laws) that are learnt via minimization of observables error and mutual information across scales. We investigate how this can guide us to formulate scaling laws and we explore means to accelerate scaling of dynamic processes and to reduce data requirements.

Poster #21-24

Assimilation of Multiscale Data into Multifidelity Biogeochemical Models

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BER Program: SBR

Project: University Award

Vast disparity of spatiotemporal scales on which data are collected and models are used remains one of the key challenges in accurate and reliable predictions of watershed dynamics. We generate multi-resolution data by developing novel regression- and neural network-based closures for averaged (watershed-scale) equations of flow and transport. Then, we introduce an information-theoretic approach that allows for seamless integration of multi-resolution data into multi-scale simulations to upscale/downscale hydraulic conductivity of heterogeneous porous formations. Available data (at either the fine- or the coarse-scale) are used to inform models at the opposite scale by setting a probabilistic equivalence between the fine and the coarse scale, with closures (parameters and/or constitutive laws) that are learnt via minimization of observables error and mutual information across scales. We investigate how this can guide us to formulate scaling laws and we explore means to accelerate scaling of dynamic processes and to reduce data requirements.

Poster #22-16

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

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Project: University Award

Subsurface sediments are heterogeneous due to burial of soil horizons and organic matter. The high concentration of sediment-associated organic matter generates zones that are “biogeochemical hotspots”. These organic-rich deposits are recognized to drive metal/radionuclide reduction and trap reduced chemical species (i.e. (Fe(II)) including contaminants such as uranium (U(IV)). Thus reduced regions play a significant role trapping contaminants preventing mobility in groundwater. The existing paradigm describes oxidation of reduced metals/radionuclides upon the influx of dissolved oxygen and/or nitrate into reduced zones. However in contrast to the existing paradigm results from prior field and laboratory results demonstrated that low concentrations of oxidants directly injected into a reduced aquifer sediments stimulated reduced conditions and a decrease in groundwater uranium concentrations. We hypothesize that the influx of low oxidant concentrations into reduced zones results in the production of dissolved organic carbon (DOC) as a result of organic carbon decomposition and/or stimulation of microbial/viral activity. Whereby, the production of DOC drives reducing conditions leading to further metal/radionuclide reduction (U immobilization). However, elevated concentrations of oxidants above a “tipping point” will drive net metal/radionuclide oxidation, resulting in an increase in aqueous U concentrations. Here a series of bioreactor based experiments amended with naturally reduced organic-rich sediment from Riverton, WY are amended with U. Experiments are ongoing to monitor carbon, iron, and uranium geochemistry as well as the microbial community. This research will identify and describe the phenomena related to oxidation and reduction of metals/radionuclides in reduced regions of aquifers upon the influx of oxidants such as dissolved oxygen and/or nitrate.

Poster #22-15

Complex Effects of Redox Reactions on the Release and Degradation of Organic Carbon

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Project: University Award

Recent studies have suggested the potential for the release of iron (Fe) oxides-bound organic carbon (OC) during dissimilatory Fe reduction (DIR). However, the extent to which different forms of Fe oxide-bound (e.g. sorbed vs. co-precipitated) OC are released during DIR has not been fully resolved. Pure ferrihydrite (Fh) and Fh-humic acid coprecipitates (Fh-HA) were inoculated with a small quantity of freshwater sediment and incubated under anoxic conditions in the presence and absence of H₂ or glucose as electron donors for DIR. Our results indicate that DIR can release loosely bound (e.g. sorbed) OC but may not from Fe oxide-OC coprecipitates.

Applying Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS), we investigated the fractionation of dissolved organic carbon (DOC) during co-precipitation with Fh in systems with C/Fe molar ratio of 0.5 and 3. Our results showed that high-molecular-weight DOC was preferentially precipitated for system with C/Fe of 3. In addition, a higher fraction of condensed polycyclic aromatic hydrocarbons (98.12%) was co-precipitated compared to unsaturated phenolic (66.25%) and aliphatic (39.01%) DOC. Our findings demonstrated that high-molecular-weight aromatic compounds preferentially co-precipitate with Fh in systems with feed C/F ratio relevant to the natural systems.

In the field, year-round measurements of ecosystem-scale methane and carbon dioxide fluxes were undertaken at Toolik Field Station in the Alaskan Arctic over two years. Year 1 cold season net carbon dioxide and methane fluxes, however, were 47 % and 150 % higher, over a shorter cold season (22 days shorter). Relationships between methane fluxes and surface temperatures were almost reversed to Year 2, though similar relationships between respiration fluxes and surface soil temperature were observed across both years. Our results suggest that high cold season methane emissions are linked to temperature thresholds in deep, active layer zones and highlight a need for measurement and modelling of soil temperatures throughout the year and entire active profile in order to better predict potential changes in the annual methane exchange budget in Arctic tundra regions.

Poster #21-23**Using Global Sensitivity Analysis to Identify Controlling Processes of Complex Systems**Ming Ye^{1*}, Gary Curtis², and Li Li³¹ Florida State University, Tallahassee, FL² U.S. Geological Survey, Menlo Park, CA³ Pennsylvania State University, State College, PAContact: mye@fsu.edu

BER Program: SBR

Project: University Award

For an open and complex environmental system, it is always difficult, if not impossible, to understand all the processes and their interactions. On the other hand, since the system dynamics are determined mainly by controlling processes, a better understanding of the controlling processes can lead to advanced predictive understanding of the system. Therefore, identifying controlling processes is always the first step for gaining predictive understanding. The identification, however, is challenging because of uncertainty inherent in system processes such as process parameters and conceptualizations. The overarching scientific question to be answered in this project is as follows: *If we are not certain about the choice of process models and model parameters, can we correctly identify the controlling processes of a complex system?* To answer this question, this project introduces the concept of multiple working hypotheses into the identification of controlling processes to explicitly take into account the uncertainty in conceptualizing and simulating individual processes.

In this poster presentation, we will first present a case study that uses sensitivity analysis to improve a nitrogen transport model developed based on the mixing layer theory. The sensitivity analysis considers three parameters, the mixing layer thickness and two mass transfer coefficients from the mixing layer, and identifies that the mixing layer thickness is the most important parameter. In other words, the nitrogen mixing process is more important than the mass transfer process. To improve the nitrogen transport model, a time-dependent equation is derived to estimate the mixing layer thickness to replace the constant mixing layer thickness used in the conventional mixing layer theory. Using the time-dependent mixing layer thickness substantially improves the model fit to observed nitrogen concentrations in a laboratory experiment.

Another achievement made in this project is the improved computational efficiency for calculating the process sensitivity index, which is the key variable for identifying dominating processes. The calculation is based on Monte Carlo simulation, and the original way of calculation is computationally expensive because it is based on combinations of model parameter samples. We developed a new method to remove the sample combination, which reduces the number of model simulation from the order of N^2 to N , N being the number of parameter samples. We are implementing the new computational method for uranium reactive transport modeling at Naturita, which involves three processes, i.e., groundwater flow, uranium transport, and uranium surface complexation reaction. The goal is to identify the controlling processes for contaminant remediation.

Scientific User Facilities and Community Resources

EMSL: A DOE Scientific User Facility for Earth System Science Research

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BER Program: Scientific User Facility

Project: EMSL

Project Website: <http://www.emsl.pnl.gov>

Robust, predictive models of elemental cycling in terrestrial ecosystems and contaminant fate and transport in the subsurface require understanding and identification of key microbial, biogeochemical and hydrologic processes that control species reactivity and mobility across multiple spatial and temporal scales. The ability to identify and adequately probe dynamic processes at the molecular to pore scale provides mechanistic information needed to accurately represent these processes in computational reactive flow and transport models, an important goal of many Environmental System Sciences researchers who address the nation's environmental and energy challenges. Linking experimental and theoretical approaches from molecular to field scale requires the convergence of diverse experimental and computational techniques and collaboration with experts from multiple disciplines.

EMSL, a DOE national user facility in Richland WA, provides integrated experimental, computational, and modeling and simulation resources and expertise for scientific studies and discovery in Earth Systems Science to users free of charge. There are numerous capability sets that are particularly relevant for such research. I) Next generation imaging and surface characterization experimental capabilities can be used to provide the spatially resolved elemental analysis, oxidation state determination, chemical speciation, mineral identification, and microbe-mineral associations necessary for understanding the chemical fate and mobility of contaminants in the biogeochemical environment or microbial communities and nutrient cycling in the rhizosphere. II) Advanced spectroscopic capabilities are used for determining the speciation of metal ions and complexes on surfaces, in solution, or incorporated into mineral phases. III) A comprehensive suite of mass spectrometry platforms for proteomics/metabolomics, whole transcriptome analysis, gene expression profiling, small RNA analysis, novel transcript identification, and many genome- and epigenome-directed applications provide EMSL users extensive capabilities for unraveling the interplay between microbes, plants, soil, and geochemistry. IV) An integrated suite of capabilities to support research in subsurface flow and transport provide data from the micron to the intermediate scale. Experts assist users with pre-experiment modeling to hydraulic characterization, numerical modeling, and post-process analysis on custom-built flowcells. V) EMSL's Plant Ecosystem Lab offers different types of plant growth facilities including Conviron walk-in rooms and Percival chambers. This allows growing and investigating plants under environmentally controlled conditions with defined temperature, humidity, light intensity, and CO₂ levels. EMSL is expanding capabilities to couple computational resources with data generation: we are coupling metabolomics measurements with NWChem molecular dynamics simulations to achieve "standards-free" accurate identification of metabolites thereby expanding the number and diversity of metabolites identified by mass spectrometry and we are performing genomic sequence analysis and data mining to improve the depth of coverage from proteomics studies. The extensive expertise at EMSL in multi-scale reactive transport modeling spans the pore-to-basin scale; in particular, our modeling expertise encompasses experience with a diverse suite of software systems, including SPH and TETHYS for pore-scale simulation and PFLOTRAN, Amanzi and eSTOMP for continuum-scale simulation.

JGI: Genomic Resources for Advancing Environmental System Science

Esther Singer^{1*}

¹Joint Genome Institute

BER Program: Scientific User Facility

Project: JGI

Project Website: <https://jgi.doe.gov/>

As a User Facility, in fiscal year 2018 the JGI served a worldwide community of 1,882 users from academia, government, and industry generating more than 178 trillion nucleotides of genome-sequence data from microbes and microbial communities, fungi, algae, and plants. In support of these projects, JGI produced 53 plant genome annotations and 2,190 resequenced plant genomes, 222 annotated fungal genomes and 2,557 microbial genomes (including single-cells), as well as 1,898 metagenomic data sets. As we continue to advance our functional genomics, we generated 2,994 plant transcriptomic and 692 metatranscriptomic datasets. In total this led the JGI to produce a record sequencing output of 225 trillion bases of sequence data in FY18.

The JGI generated 232 publications in peer-reviewed journals. In addition, data from sequencing projects are disseminated to the broader scientific community via the JGI's data portals. There were more than 11,000 new data users in FY18.

New Pipeline for Multi-omics Data Integration and Discovery in KBase to Identify the Mechanism Driving Metabolic/OTU Dynamics in a Microbiome

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Project Website: <http://kbase.us>

Project Goals: The Department of Energy Systems Biology Knowledgebase (KBase) is a knowledge creation and discovery environment designed for both biologists and bioinformaticians. KBase integrates a large variety of data and analysis tools, from DOE and other public services, into an easy-to-use platform that leverages scalable computing infrastructure to perform sophisticated systems biology analyses. KBase is a freely available and developer extensible platform that enables scientists to analyze their own data within the context of public data and share their findings across the system.

Increasingly microbiome systems are being interrogated using a combination of DNA sequencing and metabolome mass spectrometry with the ultimate goal of understanding how microbial communities shape (and are shaped by) the chemistry of their surrounding environments. Yet, the challenge of deciphering the biological mechanisms that give rise to observed dynamics in metabolite and species abundances in a given environment based on this data remains. Here we demonstrate a new workflow in KBase, comprised of many new data types and tools recently added to the KBase platform that permit users to:

- (1) identify metabolites and species that correlate based on cross-comparison of samples;
- (2) search for isolates of species of interest that interact with metabolites of interest;
- (3) predict biosynthesis pathways for a metabolite of interest in an isolate of interest;
- (4) identify gene candidates for gap-filled steps within a predicted pathway;
- (5) check phylogenetic neighbor genomes for evidence of conservation of pathway of interest;
- (6) find and query available transcriptomes for evidence of expression of pathway of interest;
- (7) identify other environments that involve similar species, metabolites, and pathways.

We demonstrate this new pipeline in action by analyzing a dataset from the Ecosystems and Networks Integrated with Genes and Molecular Assemblies (ENIGMA) SFA. In this study, a soil core was retrieved from a contaminated aquifer at the Oak Ridge National Lab Field Research Center (ORNL FRC), and fourteen biological samples were collected from this core at 9 inch vertical intervals. Each sample underwent both amplicon sequencing and metabolomic analysis, identifying a total of 3940 OTUs and 34 metabolites. Within KBase, we were able to correlate the OTUs to the metabolites. As we were particularly interested in applying a multi-omics approach mechanistically to understand these correlations, we applied the *Object Counts by Taxon* tool, which leverage the KBase Relation Engine that connects together related data entities in KBase, to identify which taxons in our dataset had the most multi-omics data available elsewhere in KBase. In this analysis, *Pseudomonas* emerged as the best candidate. Of the metabolites correlated to *Pseudomonas*, betaine had highest positive correlation. A search in KBase revealed the Web of Microbes dataset uploaded by the Northern lab as part of a JGI collaboration with KBase, which demonstrated that a particular isolate of *Pseudomonas* is known to produce betaine as a byproduct. We applied the *Predict metabolite biosynthesis pathway* tool in KBase to identify 17 reactions and 30 genes involved in betaine biosynthesis in this strain of *Pseudomonas*, with three of the reactions having unknown genes (including the final step in betaine biosynthesis). We applied the *Find Candidate Genes for a Reaction* tool, which is another tool that leverages the KBase relation engine, to identify candidate genes for each of the three gap-filled steps in the betaine pathway. We then used the *Homolog Genome Context* to study how conserved all the betaine pathway genes (including our new candidate genes) are across all close *Pseudomonas* genomes. Close *Pseudomonas* genomes were determined using the *Mash Search* tool in KBase, which was developed in

collaboration with JGI. This analysis revealed that the betaine pathway is broadly conserved in *Pseudomonas* genomes. We used data discovery tools (driven by the relation engine) in KBase to identify numerous public transcriptome profiles for some of the close *Pseudomonas* genomes identified by MASH. A search of our betaine gene families in these datasets revealed that they are most often expressed in antibiotic and protozoa induced stress conditions. Finally, we applied the *MAG (Metagenomic Assembled Genomes) Mash* tool, which was also developed in collaboration with JGI, to identify metagenome samples that contain similar *pseudomonas* genomes, revealing other environments where *Pseudomonas* and betaine production are potentially significant.

Overall, using the data discovery and analysis tools in KBase (and less than one hour of user-time), we were able to develop a mechanistic explanation for a metabolite-OTU correlation, identify missing genes in the betaine biosynthesis pathway in *pseudomonas*, determine that the betaine pathway is highly conserved in *pseudomonas*, pinpoint some conditions under which the betaine pathway is expressed, and explore some other environments where similar genomes are known to exist. The combination of tools applied in this workflow can be used to perform similar studies on numerous other microbiome and isolate systems, enabling the integration of multi-omics data to translate correlation to mechanistic understanding.

Reference:

KBase is funded by the Genomic Science program within the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research under award numbers DE-AC02-05CH11231, DE-AC02-06CH11357, DE-AC05-00OR22725, and DE-AC02-98CH10886.

Small Business Innovative Research (SBIR) Awards

Poster #21-54**Long-Term, Real-Time Monitoring of Water and Sediments using Microbial Sensors**

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BER Program: SBR

Project: SBIR

A novel sensor system was developed allowing long-term monitoring of natural and man-made environments. The monitoring system measures the potential difference between the biofilm populating the surface of an inert electrode and a reference electrode. The system has several very significant advantages including: 1) large sensor arrays can be deployed in the field, 2) the sensors require no maintenance or calibration, and 3) the sensors may be deployed in natural waters, saturated or unsaturated environments, allowing monitoring of diverse environments.

The sensors are interfaced with signal/communication (cellular) electronics to allow real-time data collection and storage of the data in cloud-based storage systems. The system has been successfully deployed in natural environments (rivers, ponds), wastewater treatment facilities, contaminated aquifers and aquaculture.

Poster #21-10**Transient Anoxic Micro-zone Development in an Alpine Stream**

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BER Program: SBIR

Project: SBIR

Project Website: <http://www.optio2.com>

Biogeochemical processes in the hyporheic zone occur over a broad range of temporal and spatial scales. The experimental challenge lies in how to obtain in-situ and time-resolved data at these different scales from a remote field site. We present spatially resolved profiles of dissolved oxygen (DO) concentration and temperature at a resolution of one data point every five minutes over an entire hydrological year from the hyporheic zone of a snow-dominated sub-alpine stream in the East River watershed in southwestern Colorado, USA (the primary site of the Watershed Function Scientific Focus Area of Berkeley Lab). We obtained these datasets from an array of novel DO sensors developed by OptiO2, LLC. The probes were located in the stream as well as buried within the streambed sediment, data being telemetered in real-time from the remote study site over a 15 month-long period. A time-lapse analysis of the oxygen profiles reveals the appearance and disappearance of anoxic micro-zones at the centimeter scale within the stream bed. Results suggest that the anoxic micro-zones move vertically over periods of days driven by processes such as snow melt and precipitation. These coupled hydrological processes lead to lateral flow in the hyporheic zone, representing a time-varying respiration contribution to the river.

We geocoded and analyzed these in-situ measurements of oxygen and temperature using spectral frequency analysis. The data were then used in a flow and reactive transport model with a Bayesian inversion procedure to predict coupled stream and hyporheic zone respiration. Specifically, we constructed a fully-coupled saturated/unsaturated flow and reactive transport model for the 2D riverbed hyporheic zone using the code MIN3P. An interesting finding from the oxygen data with depth is the observation of declining then increasing oxygen concentrations with depth. We hypothesized this was due to turbulence pressure conditions and the inclusion of sediment heterogeneity. We incorporated the role of turbulence by simulating the pressure head boundary condition as a function of Reynolds number for the river. Additionally, we included stochastic geostatistical representations of sediment parameters. Results indicate turbulence is an important metric to consider for correctly simulating subsurface redox conditions.

The data from the novel OptiO2 sensors highlight the transient behavior of anoxic micro-zones in the context of an unusual snow drought hydrological cycle. Efforts are underway to use these high-resolution oxygen and temperature data in mechanistic models to enhance process understanding in stream beds and hyporheic zones.

Poster #21-1**From Data to Models and Analytics: An Integrated Scientific Computing Platform to Accelerate Environmental Research**

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Advances in sensor-based field observations, multi-scale models, and computational technologies in Environmental Systems Science (ESS) provide new opportunities for applied research and development in academia and industry. These same advances are producing spatially and temporally heterogeneous data of growing size with different measurement frequencies and increasingly varying types and formats. As a result, current and foreseen model-data integration efforts require handling wide varieties and large volumes of data for pre-processing, simulation run, and post-processing which consequently requires the use of complex technologies such as data and resource management, high performance (HPC) and cloud computing. However, current tools and efforts for model-data integration in the ESS domain lack turnkey solutions for model-data integration workflows that involve large and complex data management, scalable pre and post-processing, and a complete suite of scientific visualization features. What makes it more challenging is that the current efforts are either fragmented or specialized for one-off systems. To reduce this fragmentation and to provide scalable model-data integration solutions, there is a need for an integrated software platform to advance research and development using simulation models. Furthermore, there is an urgent need to rethink traditional workflows which involves moving data between resources as needed for visualization and hypothesis formulation as the data is getting larger and computing costs (both HPC and cloud) are becoming cheaper.

To address the challenges described above Kitware and its collaborators are developing an integrated open source platform, Gaia, providing turnkey solutions for model-data integration using modern web technologies, advances in HPC and cloud computing and high-performance visualization. A key feature of our platform is that it minimizes and automates data movement between data storage and computing systems. Another critical feature of our design is that it enables users to perform high-fidelity post-processing by performing high-performance visualization server-side and in-situ on the compute cluster close to the data. Gaia will use Kitware developed VTK, ParaView, Girder, and community-led Jupyter effort in a loosely coupled modular design. In Phase I, we prototyped Gaia, enabling unified data access and server-side preprocessing operations. In Phase II, we will integrate simulation codes and post-processing capabilities while continue to enhance Phase I features to achieve a production-ready platform before the end of Phase II. We will also deploy Gaia at DOE HPC and cloud systems.

Poster #21-70**Probing Biogeochemical Processes in Coastal Ecosystems with High- Resolution/Long-term Dissolved Oxygen Measurements**

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Dissolved oxygen (DO) is an indicator for the metabolic state of aquatic ecosystems, representing an integrated signal from the interface of ecosystems. The cycling of carbon and nutrients is intimately linked with DO, making it a powerful parameter for interpreting a wide- range of biogeochemical processes. However, current DO sensor technologies require frequent attention by researchers to ensure proper calibration and data logging. Here we show results from a newly developed optical DO sensor technology by OptiO₂, tested in a variety of coastal settings. First, we deployed the OptiO₂ sensor in a nearshore marine environment (Sequim Bay, WA), where salinity remains close to full-strength seawater, to test its ability to make in situ salinity corrections. Over a several week-long deployment, the OptiO₂ data was in agreement with two commercial units with the added benefit of being able to telemeter data, collect data in high-resolution (1 minute frequency) with reduced power draw, and a small sensor footprint enabling non-traditional deployment approaches. These benefits allowed us to observe real-time changes in DO in Sequim Bay linked to tidal height, with lower DO values observed at low tide. The sensor's small size enabled deployment in a novel benthic flux chamber system, which quantifies the rate of DO drawdown by sediments. Benthic flux chamber results suggest that respiration in Sequim Bay sediments consume considerable amounts of DO, perhaps accounting for decreased DO levels at low tide. We next deployed the system at the mouth of a first-order coastal stream, Beaver Creek, to test performance under dynamic salinity ranges and in belowground environments. The system consisted of a battery/solar powered data collection station that autonomously transmits the DO, temperature, salinity and atmospheric pressure data from multiple sensors over a wireless connection. Beaver Creek is completely fresh during low tide and surface waters experiencing salinities up to 30psu at high tide. Groundwater below the adjacent terrestrial landscape also experiences tidal fluctuations in water level and salinity. We deployed the OptiO₂ probes in the river and two settings inaccessible to commercial sensors—in a groundwater well and in a groundwater seep that exchanges water with Beaver Creek. Similar to Sequim Bay, surface water DO was lowest during low tide. However, we speculate that this DO variability in Beaver Creek was largely driven by differences between fresh/saline waters at low/high tide and consumption of O₂ as water moves into and out of the terrestrial landscape.

Poster #21-9**New Analytical Tools for in-situ Research of Biogeochemicals and Trace Metals**Donald Nuzzio^{1*}¹ Analytical Instrument Systems, Inc., Flemington, N.J.Contact: ais@aishome.com

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Project: SBIR

The challenge in collecting data from any environment is the lack of tools that combine all the measurements required to understand a particular system under study. Researchers are left with interfacing together a myriad of instruments to obtain the information required.

Our SBIR Phase II project has focused on bringing electrochemical instrumentation into the field in a simple, affordable and user-friendly system. From the preparation of the sensor itself, to controlling the instrument and then processing data we have put together new unique systems allowing for accurate collection of biogeochemical data from any aquatic environment. These new electrochemical systems can perform any analysis from anodic or cathodic stripping voltammetry to simple current monitoring experiments. These systems allow the detection of most biogeochemicals including (and not limited to), oxygen, sulfide, iron, iron sulfide, and manganese directly on one sensor in real time in about 3-5 seconds. Analyzing any ion in the environment from mercury to any heavy metal down to the parts per trillion levels will become routine. The design of our new instruments allow deployment into any area including rivers, streams, ponds, lakes, marshes, wells and even hydrothermal systems. A new instrument called the AIS DLK-Well-Stat-1 will be deployed at the Crested Butte area in Colorado with Ken Williams and at Savannah River National Laboratory in Aiken, South Carolina with Dan Kaplan. This particular new instrument is 1" wide and can be deployed in any well monitoring system for long periods of time. Having the ability to connect these units to telemetry will afford real time observation for any field site.

An offshoot from our basic designs has allowed us to develop an instrument called the AIS DLK MP-1, micro-pstat. This hand-held unit will allow the researcher a way to quickly investigate any water source. The above systems mentioned can be set-up and run using an iPad or iPhone as well as a simple computer interface through USB. The newly designed AIS DLK-1 instrument is a research tool allowing for more complicated integrated field measurements.

This instrument is equipped with an Ethernet connection for control and data dumping locally or to the cloud. It will also allow flexibility for mesh networks to be developed from many other instruments.

Just recently one of our DOE colleagues approached us to collect data from several sensors of their particular choice. These sensors could be easily connected to our current bench top AIS DLK-MO-1, micro-observatory system. However this system has more capability than is required for their particular application. Having a smaller more compact instrument to accomplish this, lead us to the conclusion that the AIS DLK-Well-Stat-1 could be made to collect data from any sensor (not voltammetric) with very little time in development for immediate deployments. This new instrument will be called the AIS DLK- Nano-Obs-1, and will currently allow for 4 channels of data to be collected from any analog sensor. The cost point will be less than \$1000 and allow for many systems to be deployed!!

In summary this poster will illustrate data collected from these new systems and allow the potential user insight into these new tools for research.

Poster #9-37**A Compact Ceilometer for Boundary Layer Height and Ceiling Retrievals for the Ameriflux Network**D. Sonnenfroh^{1*}, A. Richardson², and D. Albrecht²¹ Physical Sciences Inc., Andover, MA² Northern Arizona University, Flagstaff, AZContact: hchu@lbl.gov

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The advent of sensor networks to gather atmospheric data for weather and climate forecasting on large spatial and temporal scales is crucial to the advancement of our understanding of many important processes that make up such predictive models. A prime example is the height of the atmospheric boundary layer (ABL). This is an important variable as it is used to parameterize boundary layer transport in numerical weather prediction models and boundary layer effects related to fluxes and concentrations of both trace gases and aerosols in inversion models. Increased knowledge of the boundary layer structure and the diurnal evolution of its height is the goal of recent activity in Europe to establish networks of aerosol profiling lidars and ceilometers to monitor boundary layer height, as well as other parameters. The value of these networks has led to the desire to add aerosol profiling ceilometers to the AmeriFlux network, especially to aid in regional flux monitoring efforts. Given that AmeriFlux sites utilize instrumented towers, whose automated sensors are exposed to the full range of weather and must operate often with limited electrical power, a new class of laser ceilometer is needed to add boundary layer height measurement capability to the AmeriFlux network.

The height of the ABL is used as a scale length in a variety of weather and climate models to predict vertical diffusion, turbulent mixing, convective transport, and even cloud formation at the top of the ABL. Despite its value, the ABL height is not well simulated in various global climate, regional air quality, and weather forecast models. Increasing the routine spatial and temporal measurement of the ABL and cloud base heights by adding ceilometers to the Ameriflux network would provide the data needed to advance understanding of the important transport and cloud formation processes in the ABL. Such a data input would help advance the capabilities of ABL models used in weather forecasting and climate prediction. Specifically it would aid in the refinement and development of regional CO₂ flux estimates.

We are developing an ultra-compact laser ceilometer for retrievals of both ABL height and cloud base height that is compatible with the demands imposed by the wide environmental conditions experienced by, and automated operation required of, site instrumentation throughout the AmeriFlux network. For deployment at an AmeriFlux tower site, substantial reductions in size, weight, and power are needed. Compact size, a high degree of ruggedization, and thermal management with a very small available power budget are similar to design restrictions placed on aircraft and spacecraft payloads. Our design for a compact ceilometer considers thermo-mechanical stability and thermal management in the entire environmental envelope as the foundation for the sensor design. Our design approach to a laser ceilometer utilizes a fiber laser operating at a wavelength of 1.55 μ m. A fiberized transmit and receive optical train has advantages over a free space train with respect to alignment stability under varying environmental conditions. It also has advantages with respect to the size, weight and power of the sensor and enables field replacement of crucial components without disturbing critical alignment. Operation at 1.55 μ m has significant benefit for eye safe operation. The design fuses very compact fiber lasers, electronics fabrication techniques, and state-of-the-art thermal management techniques to develop a new class of ceilometer that will have the reduced size, weight, and power, as well as environmental stability, for routine, automated operation at AmeriFlux network sites.

We will review the elements of the design, including the coupled thermal, mechanical and optical modeling. We will review plans for system characterization, including accelerated thermal testing. Several engineering prototypes will undergo extensive demonstration at several AmeriFlux sites with site principal investigators.

Poster #9-35**A Compact, Broad-Band Hyperspectral SpectroRadiometer**

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A compact, robust, high-performance spectroradiometer has been developed. The system provides large signal-to-noise ratios across a broad spectral range (350-2,500 nm) and is deployable on small unmanned aerial systems. The system is based on a patented design that eliminates off-axis imaging in the fore-optics and provides an additional degree of engineering freedom as compared to conventional systems. This design results in excellent imaging and very high throughput. Test results and images are presented. Updates on deploying the instrument on a UAV with NIST will be provided.

Poster #21-55**Cloud Based Cyber Infrastructure to Enable Process Understanding**

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It is increasingly recognized that for both scientific, operational and regulatory reasons an in depth, near real time understanding of subsurface processes at thousands of sites will be required.

Obtaining such an understanding will require an enabling cyberinfrastructure which can support data collection, ingestion, management and analysis as well as collaborative research and result delivery and information use at scale. Over the last several years, through both in house funding and under multiple DOE SBIR awards and funding Subsurface Insights has developed a cloud based cyber infrastructure and associated autonomous hardware for process understanding which increasingly enables this large scale understanding.

This cyber infrastructure (PAF – Predictive Assimilation Framework) leverages open source scientific software components developed by DOE scientists (PFLOTRAN, E4D, PyFlotran), and university scientists (ODM2, PEST, Landlab). It also takes full advantage of open source frontend libraries for graphing (Plotly, D3) and user interfaces (jQuery, React) and backend tools for data analysis (e.g. Scikitlearn and R). As part of this development Subsurface Insights has been contributing to the development of several of these open source codes.

PAF has been developed and demonstrated using data from both DOE funded projects and data from other research institutions and the private sector. PAF currently can ingest geochemical, geophysical, hydrological and remote sensed data and uses the PFLOTRAN reactive transport model for modeling and analysis. Both data and capabilities within PAF can be accessed through browser and mobile interfaces and software APIs, allowing for easy integration with third party computational capabilities. An example of this is our ability to parameterize and run PFLOTRAN models both through a browser, a mobile phone and through an API.

Subsurface Insights was recently funded under a new DOE Phase I SBIR to integrate PAF with the DOE developed KBASE platform to couple microbiological and field data for enhanced subsurface process understanding. In our poster we will give an overview of the overall architecture of PAF and of the new comprehensive datamodel developed by Subsurface Insights (ODMX) which can accommodate multiple key geoscience datasets. Meeting attendees will be able to get guest accounts allowing them to run models and perform analyses.