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2017 Environmental System Science Principal Investigators Meeting

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Environmental System Science

Student Abstracts

Poster #219

Biogeochemical Fate and Stability of Iron Oxide Organic Carbon Complexes

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Associations between organic carbon (OC) and iron (Fe) minerals play an important role in regulating OC stability in the soil environment. However, Fe minerals in soil systems are subjected to redox reactions, which can compromise the stability of Fe-bound OC. Thus, understanding the process of Fe-bound OC during Fe reduction and roles of different OC functional groups is crucial for accurately predicting the C biogeochemical cycle and its response to climate change. We have systematically studied the biogeochemical fate and stability of Fe oxide-OC complexes during the abiotic and biotic reduction.

During the abiotic reduction of Fe in hematite-OC complexes, we found that the release rate for Fe bound-OC was faster than the rate of Fe reduction.¹ In addition, the aromatic OC was released during the early phase while the aliphatic OC was enriched in the residual fraction.^{1,2} The higher resistance of aliphatic OC to the reductive release provided a new mechanism for the stability of Fe-bound OC and partially explained the widely observed accumulation of aliphatic OC.

During the microbial reduction of ferrihydrite (Fh) in Fh-OC co-precipitates by *Shewanella putrefaciens* strain CN32, we found that higher C/Fe ratio of the co-precipitates facilitated Fe reduction and release of Fe-bound OC.³ The aromatic and carboxylic OC was preferentially retained in the complex during the reduction. We also investigated the fate and stability of Fh co-precipitated with model organic compounds, including glucose (GL), glucosamine (GN), tyrosine (TN), benzoquinone (BQ), amylose (AM), and alginate (AL), under anaerobic reaction.⁴ During 25-d anaerobic incubation with *Shewanella putrefaciens* CN32, Fe reduction followed the order Fh-BQ > Fh-GL > Fh-GN > Fh-TN > Fh-AL > Fh-AM. For OC release, highest OC was released from Fh-GN, and lowest OC was released from Fh-AM. OC regulated Fe reduction and consequent release of OC, through acting as an electron shuttle and regulating the bacterial activity. Effects of OC on Fe reduction were also controlled by the association and interactions of OC with Fh. These findings provided insights into the complex role of different organic functional groups in regulating the Fe reduction and stability of Fe-bound OC under anaerobic conditions.

Our results highlight that the stability of Fe oxide-OC complexes during the reduction was regulated by Fe mineral phase, the C/Fe ratio, and OC chemical composition. Such information is of great value for the development of a process-based model for prediction of biogeochemical cycles of OC.

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Poster #116

Plant Physiological Thermal Acclimation of Understory Shrubs in a Puerto Rican Tropical Rainforest.

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Tropical forests cycle more carbon than any other biome, yet there is still inadequate data to predict how these critical ecosystems will respond to Earth's warming climate. Previous research suggests that tropical species are currently operating at or near their thermal optimum temperatures and, due to the narrow temperature ranges, tropical plant species may be unable to physiologically acclimate to predicted shifts in temperature regimes. This study presents initial results of plant physiological responses to the first-ever field-level warming experiment in a tropical forest: Tropical Response to Altered Climate Experiment (TRACE). In a Puerto Rican tropical rainforest, three 4-m diameter forest understory plots were heated 4°C above mean ambient surface temperature of three control plots using infrared heaters. We tested for thermal physiological acclimation of two common understory shrub species, *Psychotria brachiata* and *Piper glabrescens*, by measuring the instantaneous photosynthetic, stomatal conductance, and respiratory responses to elevated temperatures. Pre-treatment measurements were taken in January and August of 2016, TRACE warming treatments were initiated in October 2016, and post-treatment measurements were taken in January 2017 after three months of warming. Heated plants showed evidence of acclimation, with higher photosynthetic optimal temperatures (T_{opt}); however, maximum photosynthetic rates (A_{opt}) and overall carbon uptake was lower in heated than control plants. Preliminary data suggest that the declines in photosynthesis above the optimum temperatures is due to stomatal closure. Leaf respiration rose exponentially with temperature, and preliminary data show evidence for respiratory acclimation. Results suggest that, while these plants may be acclimating by shifting their photosynthetic peaks to warmer temperatures, net CO₂ uptake may be overall suppressed or unchanged. We also present the results of a pilot study where we developed and tested a novel leaf-warming device which will be installed in the forest canopy using an access tower near the TRACE understory warming experiment in the Summer of 2017. The device successfully warms individual or groups of canopy leaves 3°C degrees above an adjacent control leaf. When combined with the understory warming experiment, we will have a synthetic mechanistic view of how both canopy and understory tropical species may respond to future, warmer temperatures.

Poster #220

The Influence of Porous Medium on Citrate Facilitated Dissolution of Uranyl-Phosphate: Connecting Batch Flow Reactors with Micromodels

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The addition of phosphate is a remediation strategy to decrease the mobility of uranium by forming a uranyl-phosphate precipitate. However, plant exudates, like citrate, can remobilize the uranium. This specific study uses batch dissolution and microfluidics experiments to examine the influence of fluid flow on citrate facilitated dissolution of uranyl-phosphate. The uranyl-phosphate was synthesized by mixing U(VI) and HPO_4^{2-} , and characterized as the mineral chernikovite ($\text{UO}_2\text{HPO}_4 \cdot 4\text{H}_2\text{O}$) with x-ray diffraction (XRD). The SEM images of the precipitate show well-defined homogeneous particles, approximately 2 μm , and the percent composition from the energy dispersive analysis corroborates the XRD results. Batch flow reactor and micromodel experiments were used to study the dissolution reaction at pH 4 with varying citrate concentrations, and the effluent was analyzed with inductively coupled plasma-mass spectrometry. The experiment used a micromodel with double inlet ports and a single outlet port with homogenous pore structures to study the impact of flow through a porous media. Raman spectroscopy and infrared spectroscopy were used to examine changes in the chernikovite over the course of the experiments.

The batch flow reactor experiments reveal that the citrate increases the amount of dissolved uranium by a factor greater than 25 with greater dissolution at longer residence times and higher citrate concentrations. After the addition of citrate to the system, the concentration of dissolved uranium increases rapidly followed by a slower decrease in uranium concentration which suggests a dissolution mechanism involving defect sites and/or a surface diffusion limitation from citrate saturation of the chernikovite particle surface. For the micromodel experiments, the chernikovite was formed in situ, precipitated down the center mixing line, and identified using Raman spectroscopy. Despite identical procedures, the size and morphology of the chernikovite precipitate that formed in the micromodels varied which impacts the dissolution of uranium. The dissolution in the micromodel experiments agrees with the trends observed in the batch flow reactor experiments, with the concentration of uranium in solution increasing with increasing citrate concentrations and with the initial increase of uranium in solution followed by the decrease. Although the micromodel dissolution experiments have much faster residence times, the concentration of uranium in solution is comparable to the concentration results from the batch flow reactor experiments with a maximum of 42 ppm in 10 mM citrate and 7 ppm in 0.1 mM citrate. This suggests that the dissolution reaction kinetics are sufficiently fast so that the shorter residence time in the micromodel does not impede the reaction. Changes in the UO_2^{+2} 870 cm^{-1} peak in the Raman spectra and the IR spectra peaks in the 1050-930 cm^{-1} range were observed between the chernikovite not exposed to citrate and the precipitate remaining after the dissolution experiments which possibly indicates a loss of structure during dissolution.

This study contributes to the larger project by providing kinetics data that will be used in studies examining the mobilization and uptake of uranium by plants. Because the micromodel is a controlled system, it is an ideal tool to isolate and study specific physical characteristics and chemical conditions. Therefore, the micromodel experiments provide a unique link between the chemistry observed in batch solution experiments and the release of radionuclides in column and field lysimeter experiments.

Poster #117

A Little Help From Your Friends: Heterogeneity in Forest Diversity Explains Observed Variation in Carbon Respiration in a Lowland Tropical Forest

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Plant roots, their associated mycorrhizal community, and the free-living microbial community interact to regulate the movement of carbon from soil to the atmosphere. Although the inclusion of plant and microbial activity in to global carbon models has generally improved model predictions, model uncertainty is still high in areas with high plant diversity and habitat heterogeneity, such as tropical forests. Heterogeneity in plant species diversity and density may create carbon decomposition hot- and cold-spots around a focal individual, leading to high measurement variation within a site. To understand how tree diversity and habitat heterogeneity influenced variation in ¹³C-labelled substrate respiration and microbial activity in a lowland tropical forest (La Selva Biological Station, Costa Rica), we first measured variation in carbon respiration rates under functionally disparate, dominant tree species, *Pentaclethra maculosa* (a nitrogen fixer), and *Goethalsia maiantha*. Additionally, to understand how free-living microbes, root-associated fungi, and plant roots shape carbon respiration, we manipulated the access of roots and mycorrhizal fungi to bulk soils *in situ*. Next, we tested how surrounding community alpha and functional diversity, shape the presence of roots, mycorrhizal fungi, free-living microbial community, and soil carbon decomposition underneath our focal individuals. We predicted that as tree community functional diversity increases around a focal individual, we would observe higher total root growth, root associated fungi, free-living microbial communities and higher variation in carbon respiration. Additionally, we predicted that carbon respiration would be suppressed around trees surrounded by a high number of con-specific neighbors.

The overwhelming variability in carbon fluxes in a lowland tropical forest was resolved when we considered a tree's neighbors. Soil respiration was highly variable throughout our study site. Despite low nutrient availability in tropical soils, we found no effect of a nitrogen-fixing tree species on organic matter decomposition. Without accounting for neighbor diversity, we detected no differences in carbon respiration among root and mycorrhizal hyphal exclusion treatments or between tree types. However, a significant amount of respiration variation was explained by variability in tree neighbor identity and diversity. Additionally, the abundance of root fungi in a focal tree was explained by tree neighbor density. Our study demonstrates that predicting carbon fluxes across diverse tropical ecosystems requires an understanding and incorporation of the diversity and functioning of the supporting plant community.

Poster #221

An Integrated Method for Molecular Investigation of Soil Organic Carbon Composition, Variability, and Spatial Distribution Across a Sub-alpine Catchment

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Cycling of carbon through soils, the largest actively cycling terrestrial carbon reservoir, is one of the more poorly constrained components of the global carbon cycle. Although soil carbon models generally represent soil organic carbon (SOC) dynamics in terms of molecular lability and recalcitrance, recent investigations suggest other processes, such as organic-mineral associations and aggregate protection, may dominate SOC turnover rates, complicating responses to climate change. As a consequence, mechanistically based soil carbon models may produce results more aligned with observations of the carbon cycle. Constructing mechanistic model frameworks requires knowledge of SOC composition at a molecular-level, yet robust characterization of SOC compositions has proven challenging. Thus, in order to reduce the uncertainty in model predictions of the land-surface response to climate change, there is a pressing need to develop advanced methods for SOC characterization and to pair these strategies with development of new model frameworks.

I have developed a novel integrated methodology using Fourier transform infrared spectroscopy (FT-IR) and bulk carbon X-ray absorption spectroscopy (XAS) to identify SOC functional groups and elemental analysis (EA) to constrain the total available SOC so that we can study SOC composition quantitatively. I am responsible for IR, XAS and EA data collection, developing the algorithm for quantifying various SOC species, and using this method to study SOC variations across the sub-alpine catchment of East River, a shaledominated watershed located near Crested Butte, Colorado. I compared the differences in the amount of various SOC species between soils from two hillslope meadows located at different elevations and life zones (upper montane at Bradley Creek, and upper subalpine at Rock Creek) and a low-lying toe-slope soil dominated by willow (Bradley Creek). At Bradley Creek, polysaccharide, traditionally considered to be labile to microbial decomposition, is a significant portion of SOC while the aromatic class (*i.e.* aromatic, quinoic, and phenolic carbon), traditionally categorized as recalcitrant, is only present in a very small amount relative to litter inputs. At Rock Creek, a large amount of carbonyl and phenolic carbon is observed, possibly due to incomplete oxidation of other SOC species. Aliphatic carbon consistently makes up a significant proportion of SOC at all sites. Possible explanations for variations in SOC distribution between these sites include differences in plant inputs or microbial decomposition level. Additionally, I used scanning transmission X-ray microscopy (STXM) to map the spatial distribution of different SOC species on small soil particles. I found that aromatic carbon is mostly concentrated on the edge of soil particles, leading to larger areas of exposure and greater accessibility to microbes. On the other hand, polysaccharide, amide, and aliphatic carbons are spread throughout the soil particles, resulting in lower physical accessibility relative to their volume. We hypothesize that this difference in spatial distribution possibly explains the increase in labile SOC species relative to plant litter inputs. Our results further strengthen the shifting soil carbon paradigm that molecular structure and thermostability are subordinate to physical protection in controlling SOC turnover rates. Further, our newly developed characterization method provides, for the first time, the ability to link SOC quantities to reactivity and above ground ecosystem properties. This work uniquely allows us to integrate SOC speciation data into a new generation of soil carbon models that can better predict the land-surface response to climate change.

Poster #222

Real Rivers Have Curves: Meander-Scale Field Investigation of Linkages Between Fluvial Geomorphology, Dynamic Hydrology, and Patterns of Hyporheic Exchange

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Hyporheic exchange is an essential component of stream and aquifer health worldwide. The exchange of waters controls biogeochemical reactions linked to nutrient cycling and regulates thermal properties necessary for hydrologic health and species diversity. Although the ecological significance of hyporheic exchange is well understood, an active area of research involves estimating biogeochemical potential of hyporheic exchange across river networks. However, current river-network scale models simplify fluvial sedimentology and discharge conditions and do not completely capture complex surface-groundwater interactions scaled across natural fluvial environments. Simplifications are rooted in a paucity of available hydrogeomorphic data and field observations in higher-order or unaltered settings, leading to the inherent exclusion or oversimplification of fluvial geomorphology in subsequent models. The absence of field observations of hyporheic exchange in diverse geomorphic settings and dynamic hydrologic conditions weakens the link between small-scale mechanistic observations and large-scale implicative studies of hyporheic exchange. This knowledge gap also precludes comprehensive estimates of how the effect of climate change on watershed hydrology will influence hyporheic exchange. In the East River WF-SFA we are conducting a field investigation focused on controls of fluvial geomorphology and discharge on hyporheic exchange in a natural sub-alpine setting. We are interested in quantifying how buried geomorphic features (fluvial sediment packages) affect the length of hyporheic flow paths and hyporheic residence times under changing surface- and ground-water conditions. The East River site provides an ideal natural laboratory for this research, because the river is actively meandering, allowing for observable connections between floodplain evolution and sedimentology. The hydrology is snowmelt dominated, providing end-member conditions of surface and baseflow hydrologic contributions. This research has three key components:

1. The introduction of a novel approach to mapping fluvial stratigraphy across multiple scales that combines point descriptions of floodplain sediments, ground penetrating radar (GPR) surveys, and remote sensing techniques to improve estimates of fluvial complexity in watershed-scale hyporheic models;
2. The implementation of continuous, meander-scale tracer tests under varying hydrologic conditions (peak snowmelt and baseflow) to observe changes in the magnitude and location of hyporheic exchange; and
3. The integration of floodplain sedimentology, tracer data, and hydrologic data into a flexible 3-D model of hyporheic exchange, and coupled with larger modeling efforts at the SFA.

Current interpretations of the field site's floodplain sedimentology and geomorphic evolution combine sediment descriptions, GPR surveys, and remote-sensing maps of former river channels. Two 24-hr continuous tracer tests are planned for the 2017 field season, with in-stream and intra-meander instrumentation. Combining the 3-D sedimentology, tracer data, and continuous hydrologic data will allow us to better observe the interactions between floodplain stratigraphy, groundwater gradients, and surface water discharge, and assess their interaction's effect on the magnitude and location of hyporheic exchange. The desired impact of this study is to 1) meaningfully integrate fluvial geomorphology into watershed-scale models of hyporheic exchange and 2) manipulate model hydrology to simulate various snowmelt scenarios and evaluate the impact on hyporheic exchange within the system.

Poster #223

Metabolic Constraints on Carbon Oxidation Impacting Metal Cycling and Greenhouse Gas Production

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Microbial metabolism of organic carbon has central controls on carbon dioxide and methane efflux from soils and sediments; it also has a primary influence on metal cycling and water quality. Four processes are widely believed to control the stability of carbon in soils and sediments, and thus its potential recycling to the atmosphere. These include 1) physical protection that spatially removes SOM from microbial enzymes, 2) chemical protection via stable bonds between soil minerals and SOM, 3) carbon composition, which determines whether SOM is suitable substrate for decomposition enzymes such as oxidases or hydrolases, and finally 4) climate, specifically cold climates, which can limit chemical and microbial activity due to frozen conditions. These largely physical processes allude to but don't directly capture the biochemical aspect of organic matter decomposition. Soil/sediment organic matter is utilized by microorganisms as an energy source, often as an electron donor. Reduced compounds require greater energy to break down and should not support microbial growth when coupled to low energy electron acceptors. This energetic limitation is seen in enzyme specialization, where enzymes either specialize on less complex hydrolysable compounds or else require oxygen in the case of very complex, often reduced or aromatic, compounds. Thus, whether a given compound is consumed should depend on how much energy it can provide the local microorganisms. Our work seeks to test whether microbial energetics play an important role in soil carbon cycling, and to examine the subsequent influence on metal cycling and greenhouse gas production.

Within the framework of microbial energetics, the presence or absence of oxygen is a key predictor of organic carbon decay pathways. As the most favorable electron acceptor (i.e. highest reduction potential), oxygen maximizes organisms' growth. In the absence of oxygen, alternative electron acceptors such as nitrate, sulfate, etc. are used, often in conjunction with organic matter as an electron donor. Contrary to traditional modeling assumptions, ours and other groups have recently found extensive respiration to be possible under anoxic conditions using alternative electron acceptors such as Fe(III) or nitrate. However, the extent of carbon mineralization under anaerobic conditions depends heavily on the chemistry of the carbon being respired. Furthermore, the importance of specific microbial taxa and communities for promoting SOM breakdown under low-energy (anoxic) conditions is largely unknown.

To test the role of microbial energetics and community structure in regulating carbon mineralization, we constructed flow-through reactors using soils that allow oxygen saturated water to diffuse downward through the soil column. Pore-water and solids were examined at depths corresponding to redox potential, as measured by microelectrodes. Inorganic chemical profiles confirm the establishment of a redox gradient and decreased respiration rates with depth. Carbon analysis via high-resolution mass spectrometry shows buildup of reduced carbon compounds. Near-edge X-ray absorption spectroscopy similarly indicates a loss of oxidized functional groups within the anaerobic domain. These chemical findings suggest that different redox zones lead to unique carbon mineralization pathways predicted using thermodynamic-kinetic models. Microbial DNA and RNA extracted from the different soil depths is being profiled, via metagenomics and transcriptomics, to elucidate communities responsible for carbon transformation within redox zones.

Poster #118

Bacterial Carbon-Use-Efficiency Predicted from Genome-Specific Metabolic Models Varies Phylogenetically and Correlates with Genome Traits

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Respiration by soil bacteria accounts for one of the largest fluxes of CO₂ from the land surface to the atmosphere, yet bacterial physiology and community composition are poorly represented in C cycle models. A single, constant parameter, carbon use efficiency (CUE), is often used in models to determine the partitioning of C between losses as respiration and incorporation into microbial biomass, which can ultimately enter the soil organic C pool. This parameter has a large impact on estimates and projections of soil C pool sizes and greenhouse gas emissions from soil; however, it is not well-understood how CUE varies between bacterial taxa and whether this variation makes microbial community composition an important factor in predicting C cycle fluxes.

We used a novel approach to estimate CUE for over 200 bacterial species based on genome-specific metabolic models built using the Department of Energy's Knowledgebase (kBase). In the absence of resource limitation, CUE varied widely between individual taxa, suggesting that intrinsic variation in potential CUE between taxa may be as large as that previously attributed to abiotic factors like temperature. Additionally, we observed a significant phylogenetic signal in CUE estimates and variation in these values was significantly related to genome traits, including genome size. For example, CUE declined by 4% per mega base pair (Mbp) increase in genome size. Finally, we explored the degree to which particular metabolites imposed constraint on CUE, and found that CUE responded most strongly to a subset of specific amino acids and carbohydrates, including lysine and arabinose. These findings provide a method for estimating CUE, a critical microbial physiological parameter in C cycle models, from genomic data available on the DOE's kBase. The relationships we observe here between microbial community composition, bacterial physiology, and C cycling provide a means for improving the mechanistic representation of microbial processes in C cycle models.

Poster #119

Understanding the Effects of Drought and Nutrient Deposition on Tree Growth in Tropical Dry Forests

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Tropical ecosystems experience dramatic changes in their dynamics due to climatic variability, and seasonally dry forests appear to be particularly vulnerable to this. A main reason of the apparent vulnerability of tropical dry forests is the susceptibility of its tree species to shifts in precipitation regimes. For instance, a recent drought event in our study sites in Costa Rica led to an increase in forest-wide mortality rates from 3% to 6.16% per year. At the same time, tree species responses to rainfall variability may vary as a function of environmental conditions, such as nutrient availability. As drought events increase in intensity and length within tropical regions, the accurate representation of tropical dry forests' responses to drought in dynamic vegetation models remain low. Thus, the overall goal of my doctoral dissertation is to understand the physiological mechanisms driving tropical tree species responses to drought events, in order to provide empirical data to parametrize vegetation models. Even though I am in my first year of graduate school, I have been working on this project as a technician for a year prior to starting my PhD studies with Dr. Powers at the University of Minnesota. Under the framework of our collaborative DOE funded project "Tropical Dry Forests Responses to Changing Climate and Nutrient Availability", I got involved in the design, establishment, and ongoing operation of a large experiment that manipulates rainfall and nutrients in plantation forests at the Horizontes Experimental Forestry Station, in Guanacaste, Costa Rica. This experiment will form the core of at least two of my thesis chapters. In the field site, we selected six tree species present in mixed timber plantations belonging to four functional types (DS: deciduous stem-succulent, D: deciduous, BD: brevi-deciduous and E: evergreen) described by our working group using a modelling approach. Then, we established 16 plots divided in four treatments (drought, nutrient addition, drought + nutrient and control) using 200 trees. At the same time, we apply nutrients twice per growing season as a complete fertilizer and drought is imposed as 50% through-fall exclusion by construction of large panels that route water off from the plots. We also track soil moisture at two depths (10 and 40 cm) in five locations within each of the 16 plots in order to quantify the magnitude of the treatment effects on this critical variable. Additional measurements include fine root production, canopy phenology by using leaf area index, soil respiration, tree growth and water status. Thus far, we have found a clear effect of our drought treatments in soil moisture, which confirms the effectiveness of our rainfall exclusion structures. We expect diminished effects of drought conditions on all tree species due to the interaction with nutrient additions, as a nutrient-rich environment may favor water use efficiency. At the same time, we expect smaller effects of the drought treatment in evergreen species as their resource-use conservative strategy might favor them to withstand drought stress. However, nutrients might allow other functional groups' species (DS, D & BD) to cope with changes in water availability. At the end, our work will fill out a gap in current knowledge required to increase the accurate representation of tropical dry forests in dynamic vegetation models.

Poster #120

Root Traits of the Most Common Tree Species in El Verde, Puerto Rico

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Fine roots are important for plant nutrient and water acquisition, but are understudied in tropical ecosystems. Fine-root traits are related to species phylogeny and environmental conditions. However, it is not well defined which of these traits are genetically based and which follow an environmental strategy. The goal of this study was to measure fine-root traits of the most common plant species at the El Verde Field Station in the El Yunque National Forest, Puerto Rico, and compare them across species and with leaf litter of the same species.

We collected root voucher samples from six common tree species in El Verde. We also collected leaf litter and eight soil cores from differing ridge and valley topography. We analyzed morphology, architecture, and nutrient concentrations in first, second, and third-order fine roots and compared nutrient concentrations with nutrient concentrations in leaf litter. Further, we installed in-growth cores, four in the ridge and four in the valley, in order to measure fine-root growth every 2 months.

We found that each species seems to have a particular combination of traits that differ from the others. For instance, *Dacryodes excelsa* is the species with the smallest root diameter, and the largest distribution of roots in the surface soil layers, with the highest concentration of phosphorus, and the highest branchiness. This species is among the most common in the area, along with *Prestoea montana*, which in contrast to *Dacryodes*, has the largest root diameter, highest branching ratio, and a consistent distribution of biomass throughout the 30 cm soil profile.

Root morphology, architecture, and chemistry are all likely important influences in tree nutrient acquisition, and subsequently ecosystem nutrient cycling. This research begins to explore these relationships to support improved representation of tree phosphorus acquisition in terrestrial biosphere models.

Poster #224

Developing Predictive Understanding of Metal Export from Coal Creek, CO

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The project is to understand and model biogeochemistry at the Coal Creek Watershed, which is located in the Gunnison Country and drains an area of approximately 52.8 km² in the west central Colorado. Biogeochemical reactions at the watershed release base cations (e.g. Na, K, Ca, and Mg) and nutrients (e.g. dissolved organic carbon (DOC), N, and P). The transport and export of these cations and nutrients could affect ecosystem functionality and downstream water quality. Specifically, we aim to understand 1) hydrological cycle and its response to climate at this snow-dominated mountainous watershed; 2) concentration – discharge (CQ) relationship of these solutes; 3) important ecohydrological drivers that govern solute transport and CQ behaviors; 4) soil organic carbon (SOC) and DOC processes and their roles in determining carbon cycling and solute transport.

This project includes: 1) compiling and analyzing the existing USGS field measured data and writing a manuscript focusing on hydrological controls on the transport of DOC and metals; 2) developing a model framework for a bio module bioRT, which features the microbially-driven redox reactions to model roots-microbe-soil-water interactions (e.g. DOC) at the watershed scale. Current results include: 1) spring snowmelts are major hydrological events at the Coal Creek Watershed and stream DOC concentration is highly responsive to discharge conditions, indicating a hydrological control on the DOC concentration; 2) large discharge events that occurred much less frequently contribute disproportionately higher fractions to the total annual water and DOC export. For example, the highest discharge bin (avg. 6.0 m³/s) occurred 4.5% of total time yet accounted for 37% of total annual water export and 49% of total annual DOC export; 3) contrasting CQ behaviors of dilution and enrichment are observed at the Coal Creek Watershed and groundwater is likely to exhibit both influences on the dilution and enrichment behaviors. Specifically, groundwater is an important source for stream Cl, Na, Ca, and Mg and the diluted groundwater in the wet period leads to the synchronized dilution pattern in stream concentration. Trace metals (i.e. Al, Zn, Mn, Fe, Cu, and Cd in ug/L) that originate from mine tailings and naturally-occurring deposits tend to be enriched in the organic-rich soils via soil adsorption and DOC complexation. A rising groundwater table under high flow conditions (during spring snowmelts) could intersect more shallow riparian soils and then flush out the accumulated trace metals that are previously disconnected to the stream, maintaining higher concentration of trace metals at high flow conditions and thus prompting enrichment behavior of trace metals.

Title: Identifying Controls on Carbon Exchanges in High Altitude Headwaters to Improve Representation in Earth System Models

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Abstract:

The hydrology of high-elevation, mountainous regions is poorly represented in Earth Systems Models (ESMs). In addition to regulating downstream water delivery, these ecosystems play an important role in the storage and land-atmosphere exchange of carbon and water. In an effort to resolve this hydrologic gap in ESMs, this study seeks to better understand the interactions between groundwater, carbon flux, and the lower atmosphere in these high-altitude environments through integration of field observations and model simulations.

Here we use observations from a meteorological station co-located with an eddy covariance tower in the East River Basin—a Colorado River headwaters basin, which is emblematic of other high-elevation basins. The meteorological and carbon flux data collected from these instruments over water year 2017, coupled with snow surveys, will be used to force an integrated single-column hydrologic model, ParFlow-CLM. These observations will be used to better constrain the water, carbon, and energy fluxes in the coupled land-atmosphere model to increase our understanding of high-altitude headwaters. Through obtaining more accurate and higher resolution evapotranspiration and carbon cycling data and applying it to a coupled hydrologic model, this study can lead to better representation of mountainous environments in all Earth Systems Models.

Environmental System Science

Early Career Awards

Poster #97

**Tropical Root Exudate Responses to Changing Water and Nutrients
TES Early Career Award**

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Organic matter exuded by plant roots can have major implications for carbon cycling and plant growth via effects on soil biota and chemistry. As a flux of carbon into soil, root exudates can be sequestered in soil by becoming trapped in soil aggregates or sorbed to soil minerals, they can be respired by microbes, or they can trigger increased release of C from soil via priming effects. In light of the importance and complexity of root exudation, we sought to understand how growing conditions affect exudation, and to test and refine three methods for measuring exudates.

We used a long-term field fertilization experiment in Panama, and growth chamber experiments using the Neotropical trees *Tetragastris panamensis*, *Tabebuia rosea*, and *Ochroma pyramidale*, to investigate effects of nutrients, water, and AMF on root exudation in tropical forests. We assessed treatment effects on exudation, comparing results from (1) collecting dissolved C after incubating roots in aerated water, (2) leaching soil pore water directly from a C-free soil matrix, and (3) using mesh bag “traps” filled with C-free matrix to collect exuded C.

Preliminary results from the field show that root exudation rates have a trend toward a negative relationship with stem diameter at breast height ($P = 0.08$, $R^2 = 0.14$), but no significant relationship with fertilization. We hypothesize that per-root exudation rates decrease with plant age because of developmental changes in the importance of acquiring nutrients and storing carbohydrates. Alternatively, mature trees may be able to invest exudates in nutrient uptake more efficiently than younger trees by targeting exudates more precisely to where they can deliver the greatest returns. We predict that refining field methods using results from the growth chamber experiment will allow for improved detection of root exudate responses to field treatments.

In conclusion, improved techniques are needed to better assess root exudation as a large-scale ecosystem process. We caution against the premature development of a single standard method for measuring root exudation. Instead, we emphasize that different methods illuminate meaningfully different components of root exudation, so we urge workers to carefully match methods to research questions. Finally, for phenomena as complex and subtle as root exudation, it is desirable to validate experimental results with multiple independent methods.

Poster #31

Spatiotemporal Variation in Recent (2002-2015) Browning and Greening Trends in the Arctic-Boreal Region of Western North America: Regional Differences, Post-Fire Trends, and Time-Series Effects **TES Early Career Award**

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Climate-induced changes in northern landscapes are well-documented in field and remote sensing studies, with predominant Boreal browning related to temperature-induced drought stress and insect infestation, and Arctic greening resulting from warmer and longer growing seasons. These trends have implications for the magnitude and direction of feedbacks to the regional carbon cycle and global climate systems. However, the patterns are highly variable depending upon the time increment examined; each increment depicts various ecological effects driven by climate variability. Accurate interpretation of overall, long term trends hinges on aggregate understanding of short-term fluctuations effected by diverse drivers. To better assess recent trends in browning and greening, we evaluated spatiotemporal patterns in remotely sensed vegetation indices in the Arctic and Boreal regions of western North America using time-series MODIS (MCD43B4 NBAR 1-km resolution) data for the growing season (May 17-Sept 6) 2002-2015. We calculated the annual maximum Normalized Difference Vegetation Index, as well as Tasseled Cap Greenness, Brightness, and Wetness. Recent trends were identified using the Theil-Sen slope estimation method with Mann-Kendall significance test. Marked differences separate Arctic and Boreal trends, including post-fire greening trends. While Arctic regions tend toward consistent, gradual greening related to warmer and longer growing seasons, unburned Boreal regions reflect a slight browning trend with much more stochastic variability tied with climate directly (warming, water stress) and indirectly via climate-influenced disturbance events (wildfire, insect outbreaks). A previously unreported, significant recent browning trend was also discovered at the southern end of the Arctic biome, possibly linked with shifting seasonality and early dissipation of annual sea ice. Effectively linking future regional-scale ecosystem responses with different scenarios of climate change will rely upon more detailed synthesis of these drivers and effects.

Poster #98

**Linking Meta-omics with the Microbial ENzyme Decomposition Model
TES Early Career Award**

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Microbes are increasingly included in soil carbon decomposition models, but it is widely recognized that one functional group may be insufficient to represent the diversity of substrates. Microbial metagenomics, metaproteomics, metatranscriptomics, and other related techniques provide important insight into microbial genes and activities, but it remains unclear how to include such detailed information in models of any scale. We provide a solution to this complex problem and demonstrate its application using a pilot study from the Gigante Fertilization Experiment near Barro Colorado Island, Panama. Soils were collected from control and phosphorus (P) addition plots and analyzed for metagenomics, metaproteomics, phosphatase enzyme activities, and CO₂ production during incubation experiments. Fertilized soils exhibited around 30% more CO₂ release than control soils and had greater microbial biomass than control soils. Control soils exhibited greater monophosphoesterase and diphosphoesterase activities, and had significantly more genes coding for the production of phytase, phospholipase, and exoribonuclease phosphomonoesterase than P addition soils. We also observed differences in genes for carbon decomposition and the reduction of nitrogen and sulfur, and results were consistent between metagenomic and metaproteomic analyses. We incorporated the enzyme functions, the P cycle (Yang et al. 2013, 2016), and a continuum carbon decomposition scheme into the Microbial ENzyme Decomposition model (Wang et al. 2013, 2014, 2015). Model results were able to match the patterns of CO₂ evolution in control and P addition soils, indicating the improved model provides a reasonable pathway for including meta-omic information into soil nutrient cycling models. Future work will focus on including anaerobic decomposition pathways.

Poster #115

Results of the First TES Early Career Project: Understanding and Simulating Drought-Induced Forest Mortality

TES Early Career Award

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Drought- and heat-induced forest mortality is accelerating globally but the mechanisms were unknown, so accurate simulation was nearly impossible. We developed testable theory and then implemented a drought and heat manipulation study in a pine-juniper woodland ecosystem to test hypotheses regarding the mechanisms of mortality. We subsequently developed model representations of these processes. Theory and data both suggest that drought- and heat-induced mortality is higher in larger plants and under hotter conditions, due in part to rising vapor pressure deficit with rising temperature. The mechanisms of mortality globally are frequently inter-related, and include carbon starvation, hydraulic failure, and biotic attack. Model improvements now allow representations of most of these processes. Process model and empirically-based projections both suggest SW USA will be free of conifers sometime near the year 2050, with the global temperate coniferous region following closely behind. Given the apparent similarity of processes across biomes, we suggest that predictions of future forest mortality can be simulated globally in the near future.

Poster #99

**Measurements and Modeling of Carbon Turnover Rates in Tropical Forest Soils
TES Early Career Award**

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Tropical forests account for over half of the global terrestrial carbon sink and 29% of global soil carbon. An understanding of how carbon dynamics in this system will respond to climate change is uncertain, and the lack of large data sets to extrapolate from field experiments to land surface models is limiting. We intensively sampled three forest and two soil types in the Luquillo Experimental Forest, Puerto Rico to quantify the age and carbon content in eleven pits across the forest. This dataset is compared to soils from AmeriFlux tropical forest sites in Brazil and Costa Rica to determine if carbon storage patterns are consistent across the broader Neotropical region.

We found that the Delta ¹⁴C values measured in Puerto Rico at depths below 1 meter are widely distributed, ranging from -100 to -800 per mil. This is unlike the other four tropical forest soils currently available (from Brazil and Costa Rica), which in comparison, only range from -200 to -500 per mil at similar depths. Radiocarbon ages and carbon stocks are being used to generate robust estimates of carbon turnover times using SoilR, a model for carbon transit times. Our measured data is compared to model generated data from the Community Land Model (CLM) and Accelerated Climate Model for Energy's land surface model (ALM).

Poster #30

Rain Promotes Methane Production & Methane Oxidation in a Thermokarst Bog in Interior Alaska TES Early Career Award

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Methane (CH₄) is a potent greenhouse gas, and wetlands represent the largest natural source of CH₄ to the atmosphere. However, 20-90% of generated CH₄ is oxidized to carbon dioxide before emission to the atmosphere, making CH₄ oxidation an important CH₄ sink. In a thermokarst bog located near Fairbanks, Alaska, a two-year field investigation that captured both an average year and the fourth wettest year on record revealed that rain promotes both methane production and methane oxidation. In the wet year, rainwater quickly warmed the entire bog soil profile down to at least 150 cm in depth and collapsed the temperature gradient in the top 60 cm. The warmer soil environment facilitated faster rates of methane production and methane oxidation. The greater rate of methane production in the wet year was fully explained by the warmer peat temperature using a Q₁₀ temperature coefficient. However, rates of methane oxidation in the wet year were greater than what could be attributed to warmer peat temperatures. Oxygen concentrations measured with planar optical oxygen sensors installed in the bog showed that, in addition to warming the peat, rain also oxygenated the peat surface. The delivery of oxygenated rainwater to the bog explains increased rates of methane oxidation during the wet year. These results, which indicate that energy and oxygen inputs from rainwater can increase rates of methane production and oxidation in boreal bogs, have implications for how wetland methane emissions may respond in the future to altered precipitation patterns. Advective delivery of energy and oxygen to wetland subsoils via rainwater is not currently a mechanism included in wetland methane models.

Poster #170

Hydrologic and Geomorphic Controls on Floodplain Erosion and Carbon Dynamics in a Mountainous Headwater Catchment
SBR Early Career Award

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A discrepancy between organic carbon (OC) inputs to inland waters and outputs, including delivery of OC to the oceans and off gassing to the atmosphere, has altered the perception that rivers act solely as conduits for OC. To explain this carbon deficit, studies have suggested that rivers are a net sink of OC within the geosphere. Beyond simply storing OC, rivers act as bioreactors with hotspots that facilitate the decomposition and mineralization of OC along floodplains. Both the storage and processing of carbon is tightly coupled to the physical and hydrological dynamics of river systems. River migration and flooding serve to transfer OC and sediment to and from the floodplain while seasonal and interannual variations in river hydrology control hyporheic and soil moisture conditions of the floodplain. The complex stratigraphy and microtopography of floodplains leads to strong heterogeneity in the storage and biogeochemical processing of OC in river corridors. Here we present data from a detailed study of the coupled, hydrogeomorphic dynamics and carbon cycling of the East River, Crested Butte, CO. We examine river dynamics and carbon cycling at yearly to decadal time scales using 60 years of aerial imagery, high-resolution aerial lidar data, ground surveys, extensive soil carbon sampling, surface water sampling, C:N elemental analysis, fourier transform ion cyclotron mass spectrometry, and nuclear magnetic resonance. Preliminary results suggests that (1) channel erosion and related OC flux is driven by the the duration and rate of decline of the annual hydrograph peak in snowmelt dominated systems; (2) on a yearly basis the net flux of sediment is from the floodplain to the channel, necessitating widespread overbank deposition from less frequent floods to balance fluxes to and from the floodplain; (3) seasonal downstream changes in particulate OC concentrations in the river suggest that the floodplain alternates between a source to a sink for OC to the river; (4) OC content across the floodplain varies with soil depth, distance from the channel, and is much higher in abandoned channels; (5) the OC in abandoned channels is also more decomposed compared to OC in other portions of the floodplain; (6) the decomposition of OC stored in the floodplain increases with distance downstream.

Poster #171

Towards a Mechanistic Understanding of Land-Atmosphere Interactions of Reactive Oxides of Nitrogen SBR Early Career Award

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Global soils are known to be a major source of oxides of nitrogen to the atmosphere. While these emissions have traditionally been associated with nitric oxide (NO) and nitrous oxide (N₂O), recent laboratory measurements and satellite-global model comparisons suggest that nitrous acid (HONO) and nitrogen dioxide (NO₂) may also be an important constituent of the N-budget. Unfortunately, the processes controlling these emissions are not understood due to challenges in elucidating details of the relevant abiotic and biogenic processes occurring within the terrestrial environment. This is especially true for soil microbial emissions of reactive nitrogen (e.g., NO, NO₂, and HONO)—gases that directly and indirectly affect climate by controlling the oxidative capacity of the atmosphere, lifetime of greenhouse gases, and formation rate of aerosols. In this presentation, I will discuss recent progress made in understanding the abiotic and biogenic processes that determine the sources and fate of HONO in soil. We developed a full automatic soil chamber array (for soil flux measurements) and field-tested it in a northern hardwood forest during a one-month field campaign at the University of Michigan Biological Station in July 2016. The system also featured a new chemiluminescence detector for ultra-sensitive detection of NO, NO₂, and HONO via a dual-wavelength photodissociation converter, which was also characterized during this time. In addition, flow reactor experiments were conducted in the laboratory to understand the mechanisms associated with the reduction of NO₂ on soil surfaces coated in soil organic matter. Our findings suggest that hydroquinones and benzoquinones, which are interchangeable via redox equilibria, contribute to thermal and photochemical HONO formation, respectively. The results provide further evidence that redox chemistry occurring on soil surfaces is a source of HONO to the nocturnal and daytime boundary-layer. Finally, I will describe kinetics studies using a coated wall flow reactor and surface composition studies using nano-DESI and nanoSIMS [at the Environmental Molecular Sciences Laboratory (EMSL)] to investigate the role that minerals and organic matter play in storing and releasing HONO in soil.

Poster #172

Computational Bayesian Framework for Quantification of Predictive Uncertainty in Environmental Modeling
SBR Early Career Award

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A computational Bayesian framework has been developed for quantification and reduction of uncertainty in environmental modeling. In this year of the project, we continue our research on sensitivity analysis under not only parametric uncertainty but also model uncertainty and scenario uncertainty. A new sensitivity index is developed for identifying important system processes, when the processes can be modeled by competing models due to model uncertainty. The process sensitivity index answers the question that how to select the important system processes when it is uncertain how to model the processes. This new method of sensitivity analysis should be of particular use at the early stage of model development when the process model uncertainty is the largest. We demonstrate this concept of important process identification using a synthetic model of groundwater reactive transport. We have collaborated with Anthony Walker at the Oak Ridge National Laboratory to use the process sensitivity index for his ecological modeling. In addition, we have also developed a new sensitivity index that can be used to identify important model components. Using the concept of Bayesian network, an environmental model is decomposed into various components, and the components can be grouped together for a sensitivity analysis. We have collaborated with Xingyuan Chen at the Pacific Northwest National Laboratory to apply the new sensitivity index to her modeling at the Hanford Site.

We have also made progress on computational evaluation of Bayesian evidence, which is critical for evaluating relative plausibility of multiple models (a more plausible model has larger Bayesian evidence). We develop a method called multiple one-stepping stone (MOSS) method that can improve accuracy of the Bayesian evidence calculation. This method has been demonstrated using an example of groundwater reactive transport modeling. On the other hand, to reduce the computational cost, the sparse grid methods are used to build cheap-to-evaluate surrogates of computationally demanding models. Using the surrogates, we compared several methods of evaluating the Bayesian evidence, including an improved nested sampling method. The future research will be focused on using the developed methods for a set of uranium reactive transport models developed for the Naturita Site in Colorado.

Terrestrial Ecosystem Science

University Awards

Poster #68

Inter-Annual Variability of Net and Gross Ecosystem Carbon Fluxes: A Review

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As the lifetime of regional flux networks approach twenty years, there is a growing number of papers that have published long term records (5 years or more) of net carbon fluxes between ecosystems and the atmosphere. Unanswered questions from this body of work are: 1) how variable are carbon fluxes on a year to year basis?; 2) what are the biophysical factors that may cause interannual variability and/or temporal trends in carbon fluxes?; and 3) how does the biophysical control on this variability differ by climate and ecological spaces? To address these questions, we surveyed published data from 59 sites that reported on five or more years of continuous measurements, yielding 544 site-years of data.

We found that the standard deviation of the interannual variability in net ecosystem carbon exchange ($162 \text{ gC m}^{-2} \text{ y}^{-1}$) is large relative to its population mean ($-200 \text{ gC m}^{-2} \text{ y}^{-1}$). Broad-leaved evergreen forests and crops experienced the greatest absolute variability in interannual net carbon exchange (greater than $\pm 300 \text{ gC m}^{-2} \text{ y}^{-1}$) and boreal evergreen forests and maritime wetlands were among the least variable (less than $\pm 40 \text{ gC m}^{-2} \text{ y}^{-1}$).

A disproportionate fraction of the yearly variability in net ecosystem exchange was associated with biophysical factors that modulated ecosystem photosynthesis rather than ecosystem respiration. Yet, there was appreciable and statistically significant covariance between ecosystem photosynthesis and respiration. Consequently, biophysical conditions that conspired to increase ecosystem photosynthesis to from one year to the next were associated with an increase in ecosystem respiration, and vice versa; on average, the year to year change in respiration was 40% as large as the year to year change in photosynthesis. The analysis also identified sets of ecosystems that are on the verge of switching from being carbon sinks to carbon sources. These include sites in the Arctic tundra, the evergreen forests in the Pacific northwest and some grasslands, where year to year changes in respiration are outpacing those in photosynthesis.

While a select set of climatic and ecological factors (e.g. light, rainfall, temperature, phenology) played direct and indirect roles on this variability, their impact differed conditionally, as well as by climate and ecological spaces. For example, rainfall had both positive and negative effects. Deficient rainfall caused a physiological decline in photosynthesis. Too much rain, in the humid tropics, limited photosynthesis by limiting light. In peatlands and tundra, excess precipitation limited ecosystem respiration when it raised the water table to the surface. For deciduous forests, warmer temperatures lengthened the growing season, increasing photosynthesis, but this effect also increased soil respiration.

Finally, statistical analysis was performed to evaluate the detection limit of trends; we computed the confidence intervals of trends in multi-year carbon fluxes that need to be resolved to conclude whether the differences are to be attributed to randomness or biophysical forcings. Future studies and reports on interannual variations need to consider the role of the duration of the time series on random errors when quantifying potential trends and extreme events.

Poster #69

Does Vapor Pressure Deficit Drive the Seasonality of $\delta^{13}\text{C}$ of the Net Land-Atmosphere CO_2 Exchange Across the United States?

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The seasonal pattern of the carbon isotope content ($\delta^{13}\text{C}$) of atmospheric CO_2 depends on local and non-local land-atmosphere exchange and atmospheric transport. Previous studies suggested that the $\delta^{13}\text{C}$ of the net land-atmosphere CO_2 flux (δ_{source}) varies seasonally as stomatal conductance of plants responds to vapor pressure deficit of air (VPD). We studied the variation of δ_{source} at 7 sites across the United States representing forests, grasslands, and an urban center. Using a 2-part mixing model, we calculated the seasonal δ_{source} for each site after removing background influence and, when possible, removing $\delta^{13}\text{C}$ variation of non-local sources. Compared to previous analyses, we found a reduced seasonal (April-September) variation in δ_{source} at the forest sites (0.5‰ increase). This small variation did not reflect the significant seasonal changes in VPD at these sites, providing evidence that stomatal response to VPD was not a dominant influence on the $\delta^{13}\text{C}$ of land-atmosphere exchange in these forests, and unlikely to be the cause of the global, coherent seasonal cycle in atmospheric $\delta^{13}\text{C}$. In contrast to the forest sites, grassland and urban sites had a larger seasonal variation in δ_{source} (5‰) dominated by seasonal transitions in C_3/C_4 grass productivity, and in fossil fuel emissions, respectively. Our findings were sensitive to the location used to account for atmospheric background variation within the mixing model method that determined δ_{source} . Special consideration should be given to background location depending on whether the intent is to understand site level dynamics or regional scale impacts of land-atmosphere exchange.

Poster #70

Large Historical Growth in Global Terrestrial Gross Primary Production

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Growth in terrestrial gross primary production (GPP) may provide a negative feedback for climate change. It remains uncertain, however, to what extent biogeochemical processes can suppress global GPP growth³. In consequence, model estimates of terrestrial carbon storage and carbon cycle –climate feedbacks remain poorly constrained⁴. Here we present a global, measurement-based estimate of GPP growth during the twentieth century based on long-term atmospheric carbonyl sulphide (COS) records derived from ice core, firm, and ambient air samples⁵. We interpret these records using a model that simulates changes in COS concentration due to changes in its sources and sinks, including a large sink that is related to GPP. We find that the COS record is most consistent with climate-carbon cycle model simulations that assume large GPP growth during the twentieth century ($31\% \pm 5\%$; mean \pm 95% confidence interval). While this COS analysis does not directly constrain future GPP growth it provides a global-scale benchmark for historical carbon cycle simulations.

Poster #91

Tropical Rain Forest Biogeochemistry in a Warmer World: Results From A Novel Warming Experiment in A Puerto Rico Tropical Forest

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Tropical forests represent one of the planet's most active biogeochemical engines. They account for the dominant proportion of Earth's live terrestrial plant biomass, nearly one-third of all soil carbon, and exchange more CO₂, water, and energy with the atmosphere than any other biome. In the coming decades, the tropics will experience unprecedented changes in temperature, and our understanding of how this warming will affect biogeochemical cycling remains notably poor. Given the large amounts of carbon tropical forests store and cycle, it is no surprise that our limited ability to characterize tropical forest responses to climate change may represent the largest hurdle in accurately predicting Earth's future climate. Here we describe results from the world's first tropical forest field warming experiment, where forest understory plants and soils are being warmed 4 °C above ambient temperatures (warming began in October, 2016). This Tropical Responses to Altered Climate Experiment (TRACE) was established in a rain forest in Puerto Rico to investigate the effects of increased temperature on key biological processes that control tropical forest carbon cycling, and to establish the steps that need to be taken to resolve the uncertainties surrounding tropical forest responses to warming. In this poster we will describe the experimental design, as well as the wide range of measurements being conducted. We will also present results from the initial phase of warming, including data on how increased temperatures from infrared lamp warming affected soil temperature and moisture, soil respiration rates, a suite of carbon pools, soil microbial biomass, nutrient availability, and the exchange of elements between leaf litter and soil (plant physiology data are shown in a separate poster by Kelsey Carter). These data represent a first look into tropical rain forest responses to an experimentally-warmed climate in the field, and provide exciting insight into the non-linear ways tropical biogeochemical cycles respond to climate change. Overall, we are striving to help improve Earth System Model parameterization of the pools and fluxes of water, carbon, and nutrients in tropical forested ecosystems and the data shown will highlight how these cycles are coupled and independently altered by warming.

Poster #59

Resolving Conflicting Physical and Biochemical Feedbacks to Climate in Response to Long-Term Warming

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The acceleration of global warming due to terrestrial carbon (C)-cycle feedbacks is likely to be an important, though poorly defined, component of future climate change. Both the sign and magnitude of these feedbacks in the real Earth system are still highly uncertain due to gaps in basic understanding of terrestrial ecosystem processes. This research takes advantage of an ongoing long-term soil warming experiment in which soils at the Harvard Forest LTER in Massachusetts have been heated for 24 years. By examining this long-term climate warming manipulation, this research targets two of the biggest questions in soil carbon response to climate warming: how will carbon use efficiency and physical protection of carbon altered in a warming world?

Long-term warming has caused the soil system to act as a positive feedback to climate, but our studies show microbes acting to promote negative feedbacks to climate. Over 24 years of warming has resulted in a 16% loss of the soil C in the top 60 cm of the soil, with a quarter of this loss happening in the last 5 years. This positive feedback is in contrast to evidence that microbes are promoting negative feedbacks, including increased simple (monomeric) C use efficiency (CUE) in heated compared to control plots, reduced microbial biomass, and thermal acclimation of microbial respiration. In other systems, CUE of complex C, which requires extracellular processing, tends to be lower than that for simple C. To account for the increased C lost as CO₂ with long-term warming, we expect to find that warming has decreased the CUE of complex (but not simple) C, which may account for the large loss of soil C over time. Physical protection is afforded to SOM by adhesion to mineral surfaces as well as by occlusion in aggregates, and these experiments will quantify both. We have also observed altered physical protection with long-term warming, where the SOM pool in the mineral soil is less processed in the heated compared to control plots. Modeling and sensitivity analysis will test the relative magnitude and interactions of physical protection and CUE for substrates of varying complexity, which will also be validated in lab studies of CUE of whole versus crushed aggregates. This work will improve the integration physical protection and C complexity into climate models, and scale measured biological, chemical and physical parameters to improve predictions of global C cycle feedbacks in a warmer world.

Poster #71

Confronting the Community Land Model Against Atmospheric CO₂ and Biospheric Datasets in the Western U.S.

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Forests in mountainous terrain represent a major carbon stock and potential for carbon uptake in the Western U.S. These forests are particularly vulnerable to climate change, which is expected to increase the frequency and severity of droughts, wildfires, and insect damage. Such disturbance events could weaken these forests' capacity to sequester carbon or switch them from a net carbon sink to a source. Despite the relevance of these mountain ecosystems, direct carbon flux measurements with eddy covariance towers are sparse, especially due to difficulties associated with complex topography. Land surface models, constrained by observed atmospheric CO₂ concentrations, emerge as an alternative for quantifying current carbon fluxes and projecting carbon dynamics into the future.

Here we simulate carbon fluxes and stocks in the Western U.S. with the Community Land Model, Version 4.5 (CLM), and assess the model performance against CO₂ observations at 3 mountain-top sites in the Regional Atmospheric Continuous CO₂ Network in the Rocky Mountains (Rocky RACCOON). The Stochastic Time-Inverted Lagrangian Transport Model, STILT, is used to link carbon fluxes simulated by CLM to CO₂ values at the observation sites. Meteorological fields from a high-resolution Weather Research and Forecasting (WRF) simulation are used to drive CLM and STILT during the summer of 2012, a period characterized by severe drought in the Western U.S. We also assess the performance of CLM against reference data products used in the International Land Model Benchmarking Project (ILAMB), including datasets on above ground biomass, leaf area index, and net ecosystem exchange.

Overall, the results show that CLM significantly underestimates carbon fluxes and stocks in the study region. We hypothesize that this is mainly caused by excessive soil moisture stress in the model due to poor representation of soil moisture over complex terrain that could be traced back to CLM's hydrology module and/or the atmospheric forcing data (especially precipitation and air temperature). New simulations testing the impact of different atmospheric forcing datasets on model performance will be shown.

Poster #107

Influence of Topography on Soil Respiration in the Susquehanna-Shale Hills Critical Zone Observatory

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Variation in soil temperature and moisture across hillslope topographic positions may exert strong controls on soil respiration (SR). We monitored the spatial and temporal dynamics of soil temperature, moisture and respiration for a growing season (171 days, May 14 to October 31, 2015) across a forested watershed in central Pennsylvania at the Susquehanna-Shale Hills Critical Zone Observatory. In addition to 8 automated chambers with hourly recorded data (LiCor-8100 system), we monitored 50 plots at 4 locations in each plot over the 8-ha catchment for soil respiration from 10:00 to 15:00 weekly. Cumulative season-long SR averaged $855 \pm 27 \text{ g C m}^{-2}$, and ranged from 484 to 1449 g C m^{-2} across the landscape. The valley floor exhibited higher soil moisture and lower temperature at a 5 cm depth than soil at the ridge top and mid-slope locations, but cumulative SR did not differ significantly with hillslope location. Mid-slope swale positions tended to have higher cumulative SR than other locations by about 100 g C m^{-2} . ($P = 0.196$). In most locations across the catchment, the seasonal pattern of SR was largely explained ($r^2 = 60\% - 90\%$) by a combination of soil temperature and moisture. Although topography had a relatively subtle effect on cumulative season-long SR, we did observe significant shifts in the relationship of SR with temperature depending on hillslope position. The seasonal temperature sensitivity (Q_{10}) of SR was higher in the valley floor and mid-slope swale locations ($Q_{10} = 2.69$ and 2.70 , respectively) compared to the ridge top and mid-slope planar positions ($Q_{10} = 1.91$ and 2.15 , respectively) for both weekly and hourly SR ($P < 0.01$). Our results suggest that landscape topography may modify the seasonal dynamics of SR by altering the responsiveness of SR to shifts in temperature.

Poster #51

Effects of Experimental Warming & Elevated CO₂ on Trace Gas Emissions from a Northern Minnesota Black Spruce Peatland

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High latitude peatlands contain nearly half of Earth's soil carbon pool and represent a particularly significant terrestrial carbon sink. As result of their anoxic conditions, peatlands are simultaneously a large C sink but also a major source of CH₄ to the atmosphere. The greatest rates of warming are occurring at high latitudes and warming is predicted to accelerate the loss of the C stored in peat as a result of faster rates of decomposition.

At present the magnitude and forms of C loss (i.e., CO₂ & CH₄) from boreal peatlands remain highly uncertain. In particular, to what extent will potential increases in forest productivity owing to rising atmospheric CO₂ concentration [herein eCO_{2,ATM}] offset potential losses of peat C owing to warming? To address this and other uncertainties we began measurement of CO₂ and CH₄ fluxes at the DOE-funded *Spruce and Peatland Response Under Climatic and Environmental Change* (SPRUCE) experiment in the Marcell Experimental Forest, MN. At the SPRUCE site, plants now grow at ambient & eCO_{2,ATM} [ambient, 900 ppmv] across a gradient of experimental warming (0 to +9 °C in 2.25 °C increments).

Across the previous three seasons of measurement [2014-2016], we find that experimental warming increases both CO₂ and CH₄ emissions. CH₄ production is more sensitive to warming and results in a declining peat efflux CO₂:CH₄ with increasing temperature. Experimental and seasonal warming increases the δ¹³C ratio of the respired CH₄ implying an increasing contribution by acetoclastic methanogens. Although the total quantity of CH₄ emitted from the S1 Bog is small, CH₄ accounts for >50% of the greenhouse gas emissions in the highest-warming treatments when adjusted for warming on a 100-year timescale.

Experimental CO₂ fumigation began in 2016. Despite the short duration of treatment, there is a clear fingerprint of the ¹³C-depleted CO₂ gas in the efflux of CH₄ and CO₂ at eCO_{2,ATM}. The isotopic detection is evident within ~1 week of gas initiation. Plant photosynthate is thus rapidly transferred belowground resulting in plant and microbial respiration, fermentation or decomposition of root exudations and the production of CH₄.

The results to date indicate belowground C in boreal peatlands is vulnerable to atmospheric loss with climate warming. The net radiative effect of these C emissions will depend an offset imposed by enhanced uptake and storage of C as atmospheric CO₂ concentrations continue to rise.

Poster #108

Carbon–Nutrient Economy of the Rhizosphere: Improving Biogeochemical Prediction and Scaling Feedbacks From Ecosystem to Regional Scales

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This project is developing plant-soil-microbial dynamics in large-scale terrestrial biosphere models, with particular emphasis on nutrient cycling and uptake (nitrogen and phosphorus), root exudation and priming, mycorrhizal interactions, and controls on the carbon cost of nutrient uptake. The model developments within the cutting-edge Fixation & Uptake of Nitrogen (FUN) model in the Community Land Model (CLM) are tested against data from six forests across the US that vary in mycorrhizal association, parent material, and climate; links to the ACME Land Model (ALM) will be explored. Measurements include assays of inorganic and organic nutrient uptake using quantum dots and isotopic tracers, estimates of carbon C of roots, exudates, and mycorrhizae using ingrowth cores, in-situ root incubations, and minirhizotrons coupled to base measurements of stand level C, N, and P budgets, and meteorology. A remote sensing framework is used to scale between the field measurements and the model resolution. The key science questions we seek to address, focusing primarily on temperate forests, include:

- How do belowground processes affect the spatial and temporal patterns of forest C sequestration, C–N–P cycling, and vegetation response?
- How does the C cost for plant N and P acquisition control productivity and vary between sites/regions with high versus low nutrient quality?
- To what degree does inclusion of mycorrhizae increase the ability of Earth System Models to predict land–atmosphere C fluxes across spatial and temporal scales?

The project started in the Fall of 2016, and the project team has been establishing both the experimental plots and baseline measurements, as well as the modeling and analysis structure.

Poster #27

Arctic Shrub Expansion, Plant Functional Trait Variation, and Effects on Belowground Carbon Cycling

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High latitude ecosystems store nearly one-half of the global belowground organic C pool in permafrost and overlying soils, which are projected to warm significantly by the end of the 21st century. Warming-driven release of this C could dramatically increase greenhouse gas concentrations in the atmosphere, thereby accelerating the warming. Arctic plant communities are also responding to warming, as evidenced by the widely documented increase in woody-shrub growth and “greening” across much of the Arctic tundra biome. This vegetation shift may offset or amplify warming by altering carbon cycling. The direction and magnitude of shrub effects remain highly uncertain, however, due to limited understanding of the consequences of shrub expansion for belowground carbon cycling and simplification of these relationships in models. The major shrubs expanding in the Arctic (*Betula*, *Salix*, and *Alnus*) vary widely with respect to aboveground and belowground traits (e.g., tissue production and chemistry, rooting depth, microbial symbionts), and may also exhibit substantial intraspecific variation in these traits in response to environmental conditions. Such variation is likely to have profound implications for soil carbon cycling.

We are investigating how plant functional traits respond to environmental conditions and affect belowground carbon stocks and fluxes. We will test the following hypotheses: (1) Aboveground and belowground plant functional traits are determined primarily by air temperature, but soil characteristics control trait response within a given air temperature range; (2) The response of soil organic carbon cycling to shrub expansion depends on plant functional traits, particularly root traits and microbial symbionts; and (3) Regardless of the dominant species, shrub expansion will interact with physical and chemical processes to increase the amount of stable soil organic carbon in the mineral soil. To test these hypotheses, we are quantifying relationships among aboveground and belowground plant functional traits and carbon stocks and fluxes along edaphic gradients nested within a temperature gradient in the Alaskan tundra. Using this sampling design, we are characterizing aboveground and belowground plant functional trait variation for individual shrub species, determining how aboveground and belowground traits co-vary, and evaluating relationships between plant functional traits and carbon stocks and fluxes. The results of this work will help to improve the parameterization and formulation of the Terrestrial Ecosystem Model, which will be used to evaluate how differences in plant functional traits affect carbon dynamics, and explore approaches to accounting for this variability in models.

Poster #109

Carbon Dynamics Across the Terrestrial-Aquatic Landscape of Subtropical Florida

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Low-latitude landscapes are a complex mosaic of natural ecosystems and built environments interconnected by hydrology from xeric forests to hydric wetlands which are vulnerable to land use changes and climate change. Perched on the boundary of subtropical and temperate climates, the low-relief landscapes of the central Florida peninsula are an archetype of a heterogeneous terrestrial-aquatic landscape under both natural and anthropogenic stress. Our study quantifies carbon dynamics at multiple scales along a terrestrial-aquatic ecosystem gradient in central Florida using multi-disciplinary techniques to understand pore-to-watershed movement of carbon and water. Our TES-funded effort has focused on eddy covariance (EC) measurements of CO₂, CH₄, and H₂O along a hydrologic gradient at three sites: pine flatwoods, seasonal depression marshes, and peat accumulating wetlands. Over the past three years all sites have been a terrestrial carbon sink. However, greenhouse gas contributions of methane emissions from the wetland sites have somewhat offset CO₂ sequestration of the landscape. Soil biogenic gas releases were mainly episodic and rapid, with greater emissions from herbaceous wetlands (44-56 mg C m⁻² day⁻¹) than forested wetlands (0.6-1.5 mg C m⁻² day⁻¹) based on laboratory incubations and field surveys with ground penetrating radar (GPR). Closed and open-topped chamber experiments showed increased C exchange with 2-3°C daytime warming, with a 50-60% increase in net C uptake at the depression marsh and flatwoods despite increased ecosystem respiration. While drought-induced encroachment of woody shrubs enhanced wetland carbon sequestration, evapotranspiration (ET) losses of water were elevated for wetlands potentially compromising their long-term stability in a warmer climate regime. Litter decomposition rates had a predictable inverse relationship with moisture across the ecosystem gradient, with a similar pattern of root productivity being greatest in the pine flatwoods compared to the wetland soils. The soils of these small isolated wetlands are a considerable stock of organic carbon and may play a vital role in the lateral movement of water and nutrients across terrestrial-aquatic interfaces, particularly given the seasonally pulsed precipitation regimes characteristic of low-latitude regions. Given the importance of low-latitude watersheds for regional and global carbon cycling, Earth System Models will be able to leverage our information and synergistic activities at a co-located NEON site, a nearby agricultural research site at Archbold Biological Station, and AmeriFlux supported coastal ecosystem research at Kennedy Space Center to unravel the processes and vulnerabilities of carbon cycling across a mixed-use terrestrial-aquatic landscape.

Poster #52

Microbial Response to Deep Peat Heating in SPRUCE Peatland Experiment

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Soil microbes are major drivers of soil elemental cycling, yet we lack an understanding of how temperature will affect microbial communities in situ. This is particularly pressing for ecosystems such as boreal peatlands because peatlands contain disproportionate amounts of carbon relative to the land area. Boreal regions are particularly vulnerable to changing temperature. We examined the response of peatland microbial communities to soil warming during the Deep Peat Heat experiment at the Spruce and Peatland Responses under Climatic and Environmental Change (SPRUCE) experimental research station. The Deep Peat Heat experimental design at SPRUCE includes ten 12 m-diameter enclosures that are warmed to five target temperatures (+0, +2.25, +4.5, +6.75 and +9 °C) at depths of 2–3 m. Warming was initiated between June 17 and July 2, 2014 as the electrical systems for each plot became available. Samples were collected June 3 prior to warming and September 9 after one season of warming. Bacterial community composition was studied using Illumina sequencing of the 16S and ITS primers to determine the response to deep peat warming of the total (DNA) and active (RNA) microbial communities.

Although temperature at depth (2 m) reached the target, surface warming was less intense, increasing on average < 2 °C. In general, soil bacterial and archaeal communities were more sensitive than fungi to warming manipulation. Microbial community composition significantly shifted with temperature for both the total (P= 0.009) and active (P = 0.001) prokaryotic communities. Generally, compositional changes for prokaryotes were greater in the 4.5 °C treatment than in the 9 °C treatment. Both Euryarchaeota and Firmicutes consistently decreased with warming, whereas Proteobacteria and Planctomycetes were sensitive to warming, but direction of response varied by genus. Taxa that consistently decreased in abundance with warming for both DNA and RNA included *Thermoanaerobacteraceae syntrophaceticus*, *Syntrophaceae smithella* and *Methanosarcina* sp. We did not detect changes due to warming in fungal community composition. The fungal genus *Suillus* responded strongly to warming in both active and total abundance, generally increasing in response. These results suggest sensitivity to small shifts of temperature can alter microbial populations. Ongoing studies are investigating the functional implications.

Poster #92

Understanding the Response of Photosynthetic Metabolism in Tropical Forests to Seasonal Climate Variations

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This project focuses on one of the fundamental questions in terrestrial system science and tropical forest ecology: what controls the response of photosynthesis in evergreen tropical forests to seasonal variations in climate? Photosynthesis seasonality in Amazon tropical forests simulated by state-of-the-science Earth system models largely disagrees with observations: while modeled soil hydrologic dynamics during drought spells dictate water shortage and, as a result, constrained photosynthesis, satellite-based retrievals of forest “greenness” and tower-based measurements of carbon dioxide exchange indicate that production remains nearly constant or increases during dry periods. This research addresses this paradigm by providing insights on seasonal climate-photosynthesis relations in two tropical forests of the Brazilian Amazon, across a gradient of dry season length between Manaus (with a short dry season) and Santarem (with a long dry season). The methods involve intensive field campaigns to measure physiological and hydraulic characteristics of leaves and trees, camera systems to monitor forest growth at tree crown and canopy scales, and ecohydrologic system continuously tracking water tree flows and their hydration status. The integration of individual tree responses over a range of light exposure conditions highlights temporal changes of the forest response to 2015-2016 El Nino conditions as well as variability of tree-scale carbon and water uptake strategies. Our tower-based phenology cameras showed that synchronization of new leaf growth with dry season litterfall shifts canopy composition toward younger, more light-use efficient leaves, thus explaining large seasonal increases (~27%) in ecosystem photosynthesis. Analysis of hydraulic relations in trees shows a spectrum of successfully co-existing strategies, ranging from tight control against xylem failure, to a near lack of regulation of the water flux through the stomata. These strategies also exhibit coupling with tree growth patterns and dynamics of non-structural carbohydrates, hinting the linkage between individual tree drought response and ecosystem-scale dynamics. We thus conclude that accounting for age-dependent variation among individual leaves and crowns as well as representation of hydraulic traits is necessary for reliable modeling of the seasonal dynamics of photosynthesis. The results suggest a new approach for integrating hydraulic traits and carbon-cycle dynamics, and a strategy for mapping traits to function of tropical forests in the next generation of predictive models of ecosystem dynamics.

Poster #53

A Peatland Biogeochemistry Model Development and Application to Quantify Peatland Methane Emissions and Carbon Accumulation

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A newly-developed biogeochemistry model that couples the dynamics of hydrology, soil thermal regime, and ecosystem carbon and nitrogen for peatlands and non-peatlands was applied to quantify the long-term peat carbon (C) accumulation in Alaska from the Holocene to present. Modeled hydrology, soil temperatures, carbon pools and fluxes and methane emissions are evaluated using observation data at several peatland sites in Minnesota (SPRUCE), Alaska, and Canada. The model was then applied to estimate C stocks in Alaska. Comparable with the previous estimates of 25-70 Pg C in peatlands and 13-22 Pg C in non-peatland soils within 1-m depth using peat core data, our model estimates a total of 36-63 Pg C at present, including 27-48 Pg C in peatland soils and 9-15 Pg C in non-peatland soils. Current vegetation stores 2.5-3.7 Pg C in Alaska with 0.3-0.6 Pg C in peatlands and 2.2-3.1 Pg C in non-peatlands. We find that the changes in vegetation and their distributions are the main factors to determine the spatial variations of C accumulation. Warmer summer temperature and stronger radiation seasonality, along with higher precipitation in the High Thermal Maximum and the 20th century might have resulted in the extensive peatland expansion and carbon accumulation. Currently we are applying the model to simulate the long-term C accumulation trajectory of the peatlands in Minnesota.

Poster #54

How Does Whole Ecosystem Warming of a Peatland Affect Methane Production?

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Peatlands are among Earth's most important terrestrial ecosystems due to their massive soil carbon (C) stores and significant release of methane (CH₄) into the atmosphere. Methane has a sustained-flux radiative potential 45-times greater than carbon dioxide (CO₂), and the accuracy of Earth system model projections relies on our mechanistic understanding of peatland CH₄ cycling in the context of environmental change. The objective of this study was to determine, under in situ conditions, how heating of the peat profile affects ecosystem-level anaerobic C cycling. We assessed the response of CO₂ and CH₄ production, as well as the CO₂:CH₄ ratio, in a boreal peatland following thirteen months of deep peat heating and fourteen months of subsequent whole ecosystem warming (surface and deep heating) as part of the Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) project. The study utilizes a regression-based experimental design including five temperature treatments that warmed the entire 2 m peat profile from 0 to +9 °C above ambient temperature beginning in June of 2014. Soil cores were collected at 25, 50, 75, 100, 150 and 200 cm depths from each experimental chamber at the SPRUCE site and anaerobically incubated at in situ temperatures. Rates of CO₂ and CH₄ production were then measured over the course of 1-2 weeks. Methane and CO₂ production in surface peat were positively correlated with seasonal and experimentally elevated temperature, but no consistent temperature response was observed at depth (75-200 cm) following both deep peat and whole ecosystem warming. Surface peat had greater CH₄ production rates than deeper peat, implying that the increased CH₄ emissions observed in the field were largely driven by surface peat warming. Additionally, the CO₂:CH₄ ratio was inversely correlated with temperature in the surface, indicating that surficial anaerobic respiration becomes more methanogenic with warming. While SPRUCE will continue for many years, our initial results suggest that the vast C stores at depth in peatlands are relatively unresponsive to warming and any response will be driven largely by surface peat.

Poster #55

The response of belowground carbon turnover and heterotrophic microbial communities to warming and elevated CO₂ in peatlands at the ecosystem scale.

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High latitude peatlands store approximately 1/3 of all soil carbon(C), but wetland-specific processes are underrepresented in global climate models. Using advanced analytical chemistry, ¹⁴C and ¹³C tracing, and next generation gene sequencing, this project quantifies the response of soil organic matter (SOM) storage, reactivity, and decomposition, and the functional diversity of microorganisms to climate change manipulation in peatlands. The project is being conducted at the Marcell Experimental Forest(MEF), Minnesota, where the Oak Ridge National Lab(ORNL) has established an experimental site known as Spruce and Peatland Response Under Climatic and Environmental Change(SPRUCE). In collaboration with SPRUCE investigators, new insights into peatland-specific processes will be incorporated into the land component of the Community Earth System Model to improve climate projections.

Multiple field campaigns were conducted at SPRUCE in summer 2016 to capture the whole ecosystem response after 1 year of whole-ecosystem warming and the immediate biogeochemical response, within days to weeks, after CO₂ enrichment (eCO₂) began. Samples were collected at 1 day, 1 week, 1 month, and 2 months after initiation of eCO₂ treatments and spanning the peak growing season at S1 bog. We determined the concentration and stable isotopic composition of CO₂ and CH₄, and $\delta^{13}\text{C}$ ($[\delta^{13}\text{C}_{\text{CO}_2}+1000]/[\delta^{13}\text{C}_{\text{CH}_4}+1000]$) values which are an indicator of the CH₄ production pathways. Microbial community composition was characterized using next generation sequencing of SSU rRNA genes. No substantial trends with time or treatment were observed. Our current results indicate that the large store of deep catotelm C remains resistant to anaerobic degradation under conditions that simulate future climatic warming.

Microcosm experiments were conducted with surface peat to examine the response of organic matter decomposition to extreme and prolonged changes in temperature. Microbial community abundance and composition were characterized along with the production of CO₂ and CH₄. Whereas CH₄ production rates exhibited a classic mesophilic response to temperature, CO₂ production showed a large temperature optimum in the psychrophilic range which matched the annual average peat temperature. The relative abundance of methanogenic archaea tracked well with CH₄ production rates, whereas bacterial abundance paralleled the CO₂ production rates. Our results indicate that peat microbial communities harbor distinct populations of psychrophilic and mesophilic bacteria. Prolonged exposure to extreme temperature triggered a loss of peat microbial community diversity and a major shift in community composition, with spore-forming members of the *Firmicutes* increasing in relative abundance at high temperatures. Microbial communities crashed at high temperatures similar to those observed, albeit rarely, at MEF.

Poster #56

Organic Carbon Decomposition Under Elevated Peat Warming and CO₂ Conditions at SPRUCE.

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High latitude peatlands store a globally significant reservoir of organic carbon. Microbial decomposition results in the conversion of organic carbon to CO₂ and CH₄. However, organic carbon stored in peatlands has remained sequestered in part because the anoxic cold conditions at these sites has slowed microbial decomposition of the peat. Climate change has led to disparate climate warming in northern latitudes presenting the possibility that microbial decomposition could be stimulated. Thus warming is expected to increase emissions of CO₂ and CH₄ which would create a positive climate feedback as these emission products are themselves strong greenhouse gases. Recent studies, however, suggest that warming may not be the only control on microbial decomposition in boreal peat (Wilson et al. 2016, 2017). We hypothesize that the lability or recalcitrance of the organic compounds in the peat itself may impart some resistance to microbial decomposition. To test this hypothesis we used multiple complementary analytical techniques to characterize the organic matter in peat collected from the Spruce and Peatlands Responses Under Climate and Environmental Change (SPRUCE, mnspruce.ornl.gov) site along with high resolution, both temporally and spatially, measurements of CO₂ and CH₄ production under elevated temperature and CO₂ treatments.

1Wilson, RM et al. (2016) Stability of peatland *Nature Communications*, 7, 13723

2Wilson, RM et al. (2017) *Journal of Geophysical Research: Biogeosciences*, in press.

Poster #57

Alpine Treeline Warming Experiment: Highlights from an Experimental Test of Expected Upslope Tree Range Shifts and Alpine Community Responses

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The elevational range of subalpine trees is known to be climate sensitive. Shifts in the distribution of trees with climate change are dependent on the demographic processes of recruitment, growth and mortality, which occur over decades to centuries for long-lived species. Alpine species are adapted to short growing seasons and are also climate sensitive. We established the Alpine Treeline Warming Experiment at Niwot Ridge, CO, to examine effects of climate warming on seedling physiology and tree recruitment near the lower limit of subalpine forest, at upper treeline, and in the alpine, as well as on the alpine plant community. We used infrared heaters to increase surface temperatures and to lengthen the growing season, and watered some plots to distinguish heating from soil-drying effects. We used long-term demography plot data to quantify adult tree growth and mortality. We integrated this experimental and observational data into spatially explicit demography models to assess impacts of warming on tree population sizes and distributions over time.

Across three subalpine tree species, recruitment is similarly constrained by a combination of temperature and moisture, with warming reducing recruitment in low elevation forest but not enhancing recruitment at treeline or in the alpine due to water limitations. Physiology measurements of limber pine show that it is most robust to drought, and indicate co-limitation of carbon assimilation by temperature and moisture in treeline and alpine sites. Warming exacerbates water limitation even in the alpine. Lodgepole pine is least tolerant of freezing, but had increased fall cold hardiness with warming. Population model results indicate century-long lags between the onset of climate changes and tree population establishment in the alpine due to seed limitation and low recruitment. Population growth is also sensitive to summer soil moisture, including in the alpine, suggesting that warming may not always result in upslope range shifts. We find rapid a decline in Engelmann spruce populations at low elevations due to recruitment failure. Alpine community productivity increases with warming only with summer water additions, an effect driven by forbs. Alpine species phenology is advanced with warming due to earlier snowmelt, with no effect of soil water. Our experimental and modeling results highlight effects of the critical interplay between summer water availability and temperature increases at individual, population, community, and landscape scales in high elevation ecosystems.

Poster #93

Ecophysiological Controls on Amazonian Precipitation Seasonality and Variability

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In this project, we aim to address how plant physiological processes, as assessed by fluorescence measurements and other observations, influence climate variability and precipitation over Amazonian rainforests, with a particular focus on the physiological control on deep convection triggering along a geographical water stress gradient. To achieve this goal, we have performed in situ observations, satellite and in situ data analysis, and the analysis of climate model results.

In situ measurements were developed along an atmospheric and soil water stress gradient, over three different sites in Amazon basin (Manaus site (K34), Rebio Jaru site (RBJ), Bananal site (BAN)). To understand the overall soil-plant-atmosphere system regarding water and carbon fluxes, we measured the seasonal variation of water transfer between soil and an atmosphere, mediated by plants, and the plant response to a seasonal or extreme water stress. We have developed and successfully installed a spectrometer that can measure fluorescence from both Fraunhofer lines in an optically transparent band of the atmosphere (745 – 759 nm) and the telluric O2A band (760 – 770 nm) in Manaus. Analysis of initial data demonstrates the advantage of Fraunhofer line SIF analysis: due to the atmosphere transparency in this band, the results are more robust in the face of changeable cloud cover than is the O2A band analysis. We expect to continue collecting data for several seasons to investigate how inter- and intra-annual changes in SIF correlate with other changes in plant ecophysiology.

Using novel remote-sensing based solar-induced fluorescence observations and a multivariate Granger causality technique, we showed that biosphere-atmosphere feedbacks are globally widespread and regionally strong, explaining up to 30% of precipitation and surface radiation variance. We show that Earth system models underestimate these precipitation and radiation feedbacks because they underestimate biosphere photosynthetic and water sensitivity. We also used the solar-induced fluorescence (SIF) measurements from two satellites that have different local overpass time (GOME2 – Global Ozone Monitoring Experiment-2: 09:30 am; GOSAT – Greenhouse gases Observing SATellite: 1:30 pm) to understand the broad spatial pattern of photosynthesis decline on a daily scale across the entire Amazon Basin. Our results suggest that there is mild mid-day depression of photosynthesis on the north, while the mid-day depression becomes significant on the south. We suggest that satellite SIF can reveal spatial and temporal patterns of vegetation water stress across Amazon.

We have compared CMIP5 model results of vertical moisture profiles in the Amazon with observations and found that are too dry at low levels, especially during the dry season. We are also evaluating the carbon uptake of CLM4.5, aiming to improve the CLM performance in simulating future land carbon uptake.

Poster #94

Solar-Induced Fluorescence Reveals the Water Stress in the Amazon Basin

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Water stress may cause the downregulation of vegetation photosynthesis in the Amazon. To understand the broad spatial pattern of photosynthesis decline on a daily scale across the entire Amazon Basin, we used the solar-induced fluorescence (SIF) measurements from two satellites that have different local overpass time (GOME2 – Global Ozone Monitoring Experiment-2: 09:30 am; GOSAT – Greenhouse gases Observing SATellite: 1:30 pm). We first compared SIF data with ground-based eddy covariance (EC) estimations of GPP. We found that SIF signal is linearly correlated with GPP on the inter-annual scale across the basin. The slope of the SIF-GPP relationship differs between the morning and mid-day. This finding provides us the basis to use SIF as a proxy for GPP. We then compared the morning SIF with the mid-day SIF along a water gradient (North-to-South), and the results suggest that there is mild mid-day depression of photosynthesis on the north, while the mid-day depression becomes significant on the south. We suggest that satellite SIF can reveal spatial and temporal patterns of vegetation water stress across Amazon.

Poster #110

Coastal Wetland Carbon Sequestration in a Warmer Climate

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Coastal wetlands are global hotspots of carbon storage. Marshes, mangroves and seagrass meadows account for about half of the total marine soil carbon pool and annual sequestration due to interactions among three primary factors: high rates of plant production, low rates of decomposition, and sea level rise. The future sink strength and carbon stock stability of these systems is uncertain because global change drivers such as temperature and elevated CO₂ perturb the complex biotic and abiotic feedbacks that drive high rates of soil carbon sequestration. Despite the leverage these ecosystems exert over the global carbon cycle, the dynamics of coastal wetland carbon pools are not presently represented in Earth system models.

In June 2016, we initiated an *in situ*, active, whole-ecosystem warming experiment and two integrated modeling activities focused on coastal wetlands. Our objectives were to: (i) examine interactions between warming, elevated CO₂ and inundation frequency, (ii) test the hypothesis that warming will increase both plant production and decomposition, but the net effect will be an increase in soil carbon sequestration rate, (iii) modify a well-established marsh carbon model to incorporate new insights gleaned from the experiment, and (iv) integrate aspects of the marsh carbon model into a wetland-enabled ACME model.

The experiment has a gradient design with air and soil warming treatments ranging from 0 to +5.1 °C, to a soil depth of 1.5 m. Elevated CO₂ will be crossed with the temperature treatment extremes (0, +5.1) beginning in May 2017. Replicate transects (n=3) are located in each of two plant communities yielding a plant community treatment that corresponds to changes in inundation across the wetland landscape. The heating treatment performed extremely well during the first season of operation.

Warming suppressed net ecosystem exchange of CO₂ (NEE, measured at 3-4 week intervals) at the site dominated by the C3 sedge *Schoenoplectus americanus*, but had no effect on the site dominated by the C4 species *Spartina patens* and *Distichlis spicata*. NEE suppression at the C3 site increased progressively with rising temperature treatment. The effect of temperature on the C3 community switched in Oct when warming began to increase NEE, a response that corresponded to delayed plant senescence. Because warming had no effect on ecosystem dark respiration in either community, we propose that temperature suppressed NEE by decreasing gross primary production. Mechanisms of warming-induced plant stress in this brackish ecosystem include stomatal closure due to lower vapor pressure deficit or higher soil osmotic potential, and nitrogen limitation due to increased sulfide production. These mechanisms will be investigated further in the second year of the experiment.

Warming increased CH₄ emissions from Jun-Nov in the C3 community site but had little effect on emissions from the C4 community. We propose that this effect is due to a decrease in rhizosphere CH₄ oxidation, which we are testing through analysis of stable isotopes. Early indications from this experiment are that responses to warming may cause radiative forcing in C3-dominated, but not C4-dominated, coastal wetland ecosystems.

Poster #58

Coupling Changes in Soil Respiration and Nutrient Cycling with Community Structure and Function in Long-Term Soil Warming Experiments

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In a twenty-six year soil warming experiment in a mid-latitude hardwood forest, we documented changes in soil carbon cycling to investigate the potential consequences for the climate system. We show that soil warming results in a four-phase pattern of soil organic matter decay and carbon dioxide fluxes to the atmosphere, with phases of substantial loss of soil carbon alternating with phases of no detectable loss. Several factors combine to affect the timing and magnitude of soil carbon loss and thermal acclimation. These include depletion of microbially-accessible carbon pools, reductions in microbial biomass, a shift in microbial carbon use efficiency and changes in microbial community composition. Our results support projections of a long-term, self-reinforcing carbon feedback from mid-latitude forests to the climate system as the world warms.

To test changes in community composition and activity, DNA and RNA were extracted from soil samples taken from three soil warming experiments at Harvard Forest, including the 26-year experiment, and submitted to the Department of Energy's Joint Genome Institute (JGI) for phylotyping (16S rRNA and ITS), metagenomics, and metatranscriptomics. The population of most abundant bacteria in our warming plots has declined by fourfold, yet the bacteria biomass has remained unchanged as fungal biomass has declined. Different views of the soil community structure were observed between DNA and RNA samples. Eukaryotic sequences comprise ~30% of the mRNA sequences in the organic layer and are an order of magnitude more prevalent than in metagenomic samples. The metatranscriptomic sequencing results included a diverse representation of the soil organismal community including RNA viruses, archaea, bacteria, protists, fungi, invertebrates and plants, a view of a canonical soil food web illustration. Significant decreases were detected in viral, fungal and invertebrate clades, while several bacterial clades increased. The number of differentially abundant taxa and expressed genes increased over the three age-staggered long-term forest soil warming experiments, suggesting an ongoing change in community structure and ecosystem function. Cellular and ecosystem functions have been effected with respect to warming, including those related to protein stability, selfish genetic elements, toxin resistance, and biogeochemical cycling (C, N, P, S, Fe).

Continued changes in soil respiration and nutrient cycling coupled with progressive changes in soil community structure and function with long-term experimental warming suggest the effects of rising global temperatures are unlikely to be ephemeral and will produce complex ecological feedbacks.

Poster #95

Extrapolating Carbon Dynamics of Seasonally Dry Tropical Forests Across Geographic Scales and into Future Climates: Improving Simulation Models with Empirical Observations

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BACKGROUND-- Seasonally dry tropical forests (SDTFs) experience a pronounced dry season lasting 3 to 7 months, and once accounted for approximately 40% of all tropical forest. Dry forests are understudied compared to tropical rainforests, and are poorly represented in earth system models. Thus, it is unknown whether SDTFs are uniquely vulnerable or resilient to global environmental changes including climate change and nitrogen deposition. We hypothesize that the responses of SDTFs to global change depend critically on belowground processes, but we lack empirical data to verify this.

OBJECTIVES—The objectives of this project are to quantify how above- and belowground processes mediate the responses of SDTF carbon dynamics to environmental change, and incorporate that understanding into two state-of-the-art models, ED2 and ACME. To do so, we are using an interdisciplinary approach that integrates: 1) field observations of ecosystem processes and plant functional traits across a range of dry forest sites in Costa Rica, Mexico, Puerto Rico, and Colombia, 2) forest-scale experiments that manipulate water and nutrient availability in Costa Rica, and 3) model simulations that quantify sensitivity of ecosystem carbon cycling to external forcings. Ultimately, our combined measurement and modeling approach will elucidate controls on C cycling in SDTFs and yield improved models for the global change research community.

RESULTS AND PROGRESS-- Empirical results We established a large-scale factorial nitrogen (N) and phosphorus (P) fertilization experiment in Costa Rica. We have found that belowground processes respond rapidly to fertilization, especially relationships with symbionts. Mycorrhizal colonization decreased dramatically in the N+P treatment only, while nodulation more than tripled in the +P treatment. Ongoing work includes a large-scale throughfall exclusion experiment and observations of ecosystem processes across the network of sites. Soil biogeochemical data suggest that correlations among soil N and P pools and cycling vary among sites.

Modeling results: (1) We used the Ecosystem Demography model 2 (ED2) to simulate field sites in Costa Rica spanning a soil fertility gradient. We compared simulated and observed measures of above- and belowground productivity. On long time scales, we are finding a strong potential for nitrogen limitation of plant productivity. In the model, this nitrogen limitation can be relieved in part by symbiotic nitrogen fixation and changes in microbial biomass and functioning. (2) In response to the empirical results, we are testing the parameterization of a new microbial model. (3) We developed a new leaf longevity parameterization based on both carbon optimization and hydraulic limitation.

Poster #111

Carbon and Energy: Climate-Induced Community Shifts and Dryland Feedbacks to Future Climate

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Due to their large spatial extent and responsiveness to climate fluctuation, drylands are suggested to play a dominant role in determining the inter-annual variability and overall trend of the land carbon sink. Nevertheless, our understanding of how different climatic drivers will interact to affect dryland climate feedbacks remains notably poor. While the data we do have suggest a strong potential for drylands to exceed climate thresholds and to span climatic pivot points, and for climate-induced changes to community composition to create large feedbacks to future climate, we are still missing key components of potential feedbacks and still lack a quantitative framework for predicting such change across drylands. Here we present data from a variety of timescales that show how different climate drivers (e.g., increased temperature and multiple altered precipitation treatments) affect the community composition, carbon cycling, and energy balance of a dryland on the Colorado Plateau, USA. Using automated CO₂ flux data from climate manipulation plots, a series of mesocosm studies, and novel soil microclimate sensors we developed for this purpose, we show substantial exchange of CO₂ between the atmosphere and dryland soils (including biological soil crusts) that is strongly controlled by surface soil climate conditions that would not be detected using traditional soil sensors. Our data highlight how these biocrust CO₂ fluxes are partitioned into net primary productivity and respiration, how these discrete fluxes are differentially affected by increased temperature, and how they are temporally and spatially decoupled from the fluxes of vascular plants. The data also show the strong role of biocrust community composition in determining CO₂ exchange, as well as in affecting ecosystem energy balance. In particular, our data suggest a large potential for climate- and land use-induced changes to biocrust community composition to strongly and negatively affect radiative forcing, with global implications for future climate. To scale these data, we are now developing new remote sensing methods that we hope will help the assessment of biocrust communities across spatial scales previously believed impossible. Taken together, these data represent a significant step forward in our understanding of and capacity to forecast how dryland organisms, biogeochemical cycles, and energy fluxes will respond to a range of future climates across a diverse biome.

Poster #60

Eight Years of Lessons from B4WarmED: Tree Responses to Warming and Rainfall Manipulation in a Boreal Ecotone

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The B4WarmED experiment addresses the potential for projected climate change to alter plant physiology and ecology at the boreal-temperate ecotone. The study has included several cohorts of juveniles of >12 tree species planted intermixed with native vegetation on 72 plots at two sites in northeastern Minnesota, and under two canopy conditions (open and understory). Since 2009 plots received three levels of both aboveground and belowground warming (ambient, +1.7°C, +3.4°C), and since 2012 half of the open plots received ≈45% less summer rainfall. Trees adjusted their carbon and water physiology, as well as their relations with herbivorous insects and mycorrhizal fungi.

We measured tree seedling and native herb and shrub phenology across multiple growing seasons. Warming caused earlier leaf out in spring for all tree species and later leaf senescence in fall for seasonally deciduous tree species, extending the photosynthetic growing season for all species by ≈10 and ≈20 days on average for +1.7°C and +3.4°C warming, respectively. We also saw strong interannual variation in the effect size of warming. For example, in aspen the mean advance of budburst with +3.4°C warming ranged from 2 days in 2013 to 18 days in 2012. Stronger effects of warming were seen in early compared to late springs, and this was true for naturally established herbs and shrubs, as well as planted tree juveniles. Differences among species in timing of budburst were also greater in early compared to late springs suggesting that climate change could increase asynchrony of leafing in forested communities. Warming altered the phenological synchrony of aspen and paper birch vis-à-vis forest tent caterpillars simultaneously exposed to contrasting warming regimes. Warming also influenced the composition of ectomycorrhizal species colonizing four tree species tested, but had minimal effect of mycorrhizal richness and did not increase colonization of boreal trees by fungal species more characteristic of the temperate biome.

Both warming and rainfall manipulation altered *in situ* light-saturated net photosynthesis (A_{sat}) as well as temperature-response functions and acclimation of V_{cmax} , J_{max} , and leaf dark respiration (R_{d}) of all species; with species varying in sensitivity to combinations of warming and drought. There was pronounced thermal acclimation of R_{d} in terms of both typical night temperatures and of high temperature tolerance. Acclimation was best explained by the mean prior 10-to-30 night temperatures, although species varied somewhat in this respect. Modest shifts in A_{sat} combined with strong thermal acclimation of R_{d} resulted in a positive relationship of R_{d} : A_{sat} to air and leaf temperatures, but with a much shallower slope than would have occurred without acclimation. In 2014 – 2016, we measured ≈440 A_{ci} curves in the field at 25°C for nine species across both warming and drought treatments, as well ≈300 A_{ci} curves measured for four species at three temperature levels (18, 25 and 32°C) again across contrasting treatments (warming and drought). Modest shifts were observed, but data are still being processed so final conclusions are uncertain.

Plant growth and survival were significantly influenced by warming, rainfall and their interaction. Low rainfall had more negative effects on plants in warmed than ambient temperatures, with most striking and negative responses for the boreal conifers. Temperate angiosperms were also more able to acclimate (with wider conduits and greater specific hydraulic conductivity) some hydraulic parameters to increases in temperature than were

boreal conifers, although surprisingly little shift in vulnerability of xylem to embolism was observed in relation to warming or drought across eight species tested.

In total, the results of B4WarmED help us understand and extend recent observations of temporal and spatial patterns of southern boreal ecotone responses to recent temperatures and rainfall regimes. Results are also being used to test and modify core physiological routines of land surface models such as ACME.

Poster #61

Measuring and Modeling the Size and Temporal Dynamics of Nonstructural Carbohydrate Reserves in Temperate Forest Trees

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Like all woody plants, trees store nonstructural carbohydrates (NSCs), such as sugars and starch, to use as carbon and energy sources for daily maintenance and growth needs, as well as during times of stress. Allocation of NSCs to storage is an important strategy associated with future growth and survival, and thus understanding NSC dynamics is important for predicting how woody plants, from individuals to whole forest ecosystems, may respond to global change. Yet, large knowledge gaps exist regarding the size and turnover of NSC pools as well as the representation of allocation and storage processes in models, both contributing to uncertainty in forecasts of future atmospheric CO₂ inputs by forest ecosystems.

The primary goal of our work is to provide a detailed picture of NSC storage in temperate forest trees in New England by quantifying the seasonal patterns of NSCs in various organs throughout the tree and constructing whole-tree NSC budgets. Monthly field sampling at Harvard Forest in 2014 along with subsequent laboratory analyses have allowed for the quantification of NSCs in foliage, branch, stemwood, and root tissues, which are currently being scaled up to determine whole-tree NSC budgets. In all species (red oak, red maple, paper birch, white ash, and white pine), sugar concentrations in branch tissue (3-5y) were lower in the growing season than in the dormant season, with sugar generally increasing from August to December. Starch concentrations peaked in October and then sharply declined to December, with the exception of white pine, which exhibited a maximum starch concentration in June, followed by a steady decline onward. Additionally measurements of sugars and starch in foliage, stemwood, and root tissues collected monthly in 2014 are currently being compiled to further resolve organ-specific seasonal patterns and contribute to estimates of NSC storage at the whole-tree level.

In 2015, we collected additional samples 1) to estimate turnover time (i.e. mean age) of NSCs stored in different tissues using radiocarbon analysis, and to better understand mixing between new and old NSCs, and 2) to explore the relationship between growth and NSC storage. These data will be used to constrain the representation of NSC storage in the transport resistance model. A parsimonious version of the transport resistance framework is being used to test the influence of varying representations of NSCs (i.e. single pool vs. continuously simulated concentration gradients), and thus improve on the simplistic and untested representations of NSC storage in most existing forest C models. Improving model representation of NSC storage is instrumental in predicting the capacity of trees to tolerate abiotic and biotic stressors and, more generally, it is fundamental to our ability to predict forest responses to global change.

Poster #62

The Role of Phenolic Compounds, Aromatics and Black Carbon Controls on Decomposition, GHG losses in Peatlands Along a Latitudinal Gradient from Minnesota to Peru

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The primary mechanisms responsible for peatland formation in boreal regions are typically attributed to cool and uniformly wet soil conditions that limit microbial respiration. However, outside of boreal regions peatlands are widespread and continue to accrete carbon despite higher temperature, seasonal drying of root-zone soil strata and recurring patterns of wildfire. This implies additional regulatory mechanisms constrain rates on organic matter decomposition and could be the primary controllers of carbon accretion in subtropical and tropical peatlands. We propose a dual control or “latch mechanism” model that predicts decomposition rates in subtropical and tropical peatlands are regulated by: (1) higher production of polyphenol and aromatic compounds in the litter of low-latitude shrub/tree communities than found in northern *Sphagnum/Carex* communities and (2) the selective removal of labile carbon and buildup of recalcitrant pyrogenic OM produced by frequent low-intensity wildfires in the native-fire-adapted communities. Wildfire season in southeastern peatlands occur in the late spring when vegetation is desiccated and peat soils have high moisture content. Notably, the surface soil layers are typically subjected to flash-heating with a rapid loss of soil moisture but little loss of soil organic matter (SOM). Key findings to-date include 1) a latitudinal gradient of carbohydrates and aromatic/phenolic compounds with low-latitude peat having fewer carbohydrates and greater aromaticity, which indicate that southern peat is more recalcitrant than boreal peat; 2) chronosequence of low-intensity prescribed burns and laboratory fire simulations showed lower H/C ratio, lower sugar+carbohydrate and lower klason lignin at burned sites; 3) Incubation of burned and unburned peat replicates over more than six months showed an initial pulse of CO₂, CH₄ and NO₂ emissions, but within four weeks emissions from the burned replicates dropped significantly below those unburned replicates. After accounting for small initial losses of organic matter (<10 %) during the fire simulations, thermal alteration of peat resulted in a net long-term reduction in carbon loss; 4) High phenolics in shrub peatlands have overarching control on the diversity and abundance of fungi—the predominant peat decomposer, thus directly decreasing carbon decomposition, but also shifting fungal composition from fast-growing to slow-growing species. This further decreases climatic decomposition sensitivity and stabilizes stored carbon. In this growing season, based on our current results we will further conduct indepth microbial, biological and chemical analysis to explore the underlying adaptive control mechanisms in temperate and tropical peatlands, thus further improving our phenol/black carbon model.

Poster #28

Direct Measurements of Permafrost Soil Carbon Loss in an Experimentally Warmed Tundra Ecosystem

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New estimates place 1330-1580 billion tons of soil carbon in the northern circumpolar permafrost zone, more than twice as much carbon than in the atmosphere. Permafrost thaw and the microbial decomposition of previously frozen organic carbon is considered one of the most likely positive feedbacks from terrestrial ecosystems to the atmosphere in a warmer world. 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—the Carbon in Permafrost Experimental Heating Research (CiPEHR) project—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 25-50%, and has degraded an increasing amount of surface permafrost each year of the project. Our previous reports have focused on measurements of carbon dioxide exchange as a metric of changes in ecosystem carbon storage, and these are ongoing. Here we report direct measurements of changes in soil carbon storage at the study site. Repeat soil measurements are not typically part of planned Arctic research and observation networks. This is largely because of ground subsidence that occurs as high-ice permafrost (perennially-frozen) soils begin to thaw. Physical alterations to the soil profile (ground subsidence) confound the application of traditional methods for quantifying carbon pool changes to fixed depths or using soil horizons. We overcame these issues by quantifying carbon in relation to a fixed ash content, which uses the relatively stable mineral component of soil as a metric for pool comparisons through time. Using this approach, we show a 26% loss in soil carbon over five years across both experimentally warmed and ambient tundra ecosystems at the research site. While the warming treatment had lower mean carbon pool amounts, this difference was not significantly different from changes in carbon pools in the ambient tundra. These surprisingly large losses overwhelmed increased plant biomass carbon uptake and were not fully detected by measurements of ecosystem-atmosphere carbon dioxide exchange. Assimilating experimental data into an ecosystem model indicated that

parameter adjustment was needed for the model to simulate carbon cycle dynamics under experimental warming. In particular, parameters for light use, gross primary production allocation, as well as transfer coefficients from litter to soil pools showed the greatest change, suggesting that there was acclimation in ecosystem behaviour in response to warming. This research highlights the potential to directly detect changes in the soil carbon pool of this rapidly transforming landscape, and that current methodologies for quantifying ecosystem carbon dynamics may be underestimating soil losses.

Poster #96

Hot Spots and Hot Moments: Investigating the Relationship Between Soil Redox Dynamics and Greenhouse Gas Fluxes in a Wet Tropical Forest

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Background/Question/Methods

Hot spots and hot moments of greenhouse gas (GHG) fluxes occur in ways that are difficult to predict or model. Soil oxygen and redox dynamics can be key predictors of these fluxes. We report on a research effort to determine to what extent soil redox dynamics are a driver of soil GHG fluxes from a lower montane wet tropical forest. We installed and sampled a sensor field across a topographic gradient in the Luquillo Experimental Forest, Puerto Rico. The sensor field included galvanic oxygen (O₂) sensors, temperature probes and time-domain reflectometry for moisture along topographic gradients. Seven sensors of each type were installed at 12 cm depth along a ridge to valley catena; the entire catena transect was replicated five times for a total of 105 sensors. Within the sensor field we also installed nine automated gas flux chambers randomly located in each topographic zone (ridge, slope and valley). A Cavity Ring-Down Spectroscopy (CRDS) gas analyzer was used to measure pseudo-continuous fluxes of carbon dioxide (CO₂), nitrous oxide (N₂O), and methane (CH₄). The experimental design produced a dataset with high temporal resolution of GHG fluxes, with nearly 10,000 measured fluxes. We also match those fluxes to soil O₂ concentrations, moisture and temperature at equally high temporal resolution.

Results/Conclusions

We found that 5%, 3% and 7% of CO₂, N₂O and CH₄ fluxes respectively were statistical outliers, large fluxes (either negative or positive) produced by hot spots in space or hot moments in time. Those outlier fluxes increased the mean flux of CO₂ by 25% (from 2.16 to 2.69 $\mu\text{mol}/\text{m}^2/\text{s}$), the mean flux of N₂O by 10% (from 0.10 to 0.11 $\text{nmol}/\text{m}^2/\text{s}$), and the mean flux of CH₄ by 77% (from 2.07 to 3.66 $\text{nmol}/\text{m}^2/\text{s}$). Soil moisture and O₂ availability followed distinct and robust topographic patterns, with significantly drier and more aerated soils in the upper topographic zones than in the valleys and lower topographic positions. Soil O₂ concentrations also experienced oscillations over hours, days and months. Soil O₂ concentrations were correlated positively with CO₂ fluxes (pearson's coefficient = 0.25) and negatively with N₂O and CH₄ fluxes (pearson's coefficients of -0.13 and -0.20 respectively). Finally, we further explore the potential for time series analysis and probabilistic statistical techniques to constrain predictions of GHG fluxes from soils.

Poster #112

Inducing Senescence of Fine Root Branches Under Root Windows by Steam Girdling

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The fine roots of plants are a substantial, though often underappreciated, component of ecosystem nutrient cycling. With turnover rates similar to those of leaves, and comprising an estimated 10-40% of forest net primary productivity, fine root turnover and associated nutrient cycling is a necessary component in understanding both the impact of these structures on the immediate rhizosphere, as well as ecosystem nutrient cycling at large. The pervasive and intimate relationship of plants to mycorrhizal fungi adds an additional consideration in the effort to understand the importance of fine roots in nutrient cycling.

Of particular interest is the process of root senescence. Resorption of nutrients during senescence of leaves is known to have a substantial influence on available nutrient pools. However, studies of root senescence are comparatively lacking. In leaves, the role of senescence associated genes (SAGs) in coordinating the senescence process (including resorption of as much as 70% of leaf N) is well studied. Similar genetic determination may be found in the process of nutrient resorption in roots, which carry the additional complexity of mycorrhizal associations. Loblolly pine roots have shown N levels similar to those found in needles, and the presence of ectomycorrhizal (ECM) colonization on root tips has been shown to influence the rate of decomposition. However, the fate of the mobile C and N during senescence is not known. Given the nature of the mycorrhizal relationship, it is plausible that fungi absorb mobile nutrients during root senescence.

The influences of plant genetic control and mycorrhizal association on fine root senescence are essential and tractable avenues to pursue in the effort to understand the role of fine roots in nutrient cycling. The work presented lays the groundwork for further studies that explore the fate of mobile C and N during root senescence in loblolly pine, and the influence of ECM colonization and genetic control on that outcome. This poster outlines preliminary work in this system that has demonstrated the efficiency of steam-girdling of fine roots as a non-destructive method to induce root senescence while maintaining conduits for nutrient resorption. Additionally, appropriate sampling times post-treatment implementation have been identified to maximize detection of C and N movement.

Poster #113

Wood Decomposition: Understanding Processes Regulating Carbon Transfer to Soil Carbon Pools Using FACE Wood at Multiple Scales

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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 with wood grown under the elevated CO₂ in the free-air carbon dioxide enrichment (FACE) experiment. By using that $\delta^{13}\text{C}$ signature in three species of wood from two FACE sites, we are effectively continuing the FACE experiment by using wood grown under elevated CO₂ as the key component 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 specific 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;
- c) Develop a module within the biogeochemical model Forest DNDC to improve estimates of log decomposition and wood C movement into the mineral soil.

The work will be conducted principally on the continental-scale (FWDE), where ambient and elevated CO₂ FACE logs were placed in 2011 on nine experimental forests, on representative soil types within different bioclimatic zones across the U.S. An established field-scale termite exclusion experiment provides unique capabilities to assess interaction among microbial communities and subterranean termites. Recent assays from the FWDE affirm that the $\delta^{13}\text{C}$ signature of the FACE wood can be traced into the mineral soil. We are building on the preliminary findings to establish what, biologically, is mediating the amounts of C we are tracing in soil, with specific interest in dominant fungal rot types and the role of termites. Forest DNDC will be provisioned with new capabilities to better reflect the dynamics of wood decomposition, mechanistically, thereby enhancing a proven platform for simulating forest C dynamics at multiple scales under current and future climate conditions and management scenarios.

Poster #29

Tracking the Fate of C Inputs to Arctic Tundra Soils from Roots to Rivers

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Rapid climate warming may already be driving enhanced decomposition of vast carbon (C) stocks in Arctic tundra soils. However, stimulated decomposition may also release nitrogen (N) and support increased plant productivity, potentially counteracting soil C losses. At the same time, additional plant C inputs may prime microbes to attack soil organic matter (SOM) to acquire N, resulting in net C losses. Since N acquisition strategies and traits differ among plant species, they may have different potentials to mediate climate-carbon feedbacks. We used field and laboratory experiments to quantify the interactions of biological, chemical, and physical controls on soil C stability.

Using isotope-tracing techniques, we found the magnitude of SOM priming depends on vegetation type and soil N concentrations. Under non-limiting N conditions, labile C inputs primed SOM decomposition in tussock soils, but did not prime shrub soils. If warming enhances decomposition and N availability, increasing shrub abundance may dampen soil C losses. This hypothesis was supported by results from a field tracer experiment, where labile C inputs reduced loss of native SOM stocks by increasing microbial substrate use efficiencies. The quality and mobility of C remaining in the soil solution will determine overall strength of the soil C sink. To quantify soluble C transport, we used bromide as a conservative tracer, and assessed DOM chemistry using a combination of fluorescence and solution-state nuclear magnetic resonance spectroscopy. Permafrost-influenced soils were significantly enriched in aromatic C, soluble microbial byproducts, and humic-type materials, while organic soils had higher proportions of fulvic acids. Rates of solute transport along the permafrost interface were similar to those through porous organic soils, suggesting permafrost thaw could mobilize SOM across the landscape.

Poster #114

Benchmarking and Improving Microbial-Explicit Soil Biogeochemistry Models

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Consideration of new insights into factors controlling the decomposition and formation of soil organic matter (SOM) will facilitate efforts to improve confidence in soil biogeochemical projections under global change scenarios. A new generation of models is beginning to integrate these processes, but concurrent efforts to create the analytical tools necessary to characterize and improve these models remain poorly developed. We describe three objectives that focus on data synthesis, parameter estimation, and the development of a soil biogeochemical testbed that can be used to investigate global SOM dynamics.

Our first objective is to synthesize a global data set relating plant input chemistry to SOM properties. Mounting research emphasizes the potential importance of litter quality in influencing the stability and chemistry of SOM. Accordingly, many soil models make predictions about how differences in litter quality drive soil C dynamics. Yet, evidence for evaluating hypotheses about litter quality effects on SOM is mostly limited to laboratory experiments and individual field studies. Our goal is to develop a data set that can be used not only for validating global-scale models, but also for evaluating our emerging hypotheses about how plant litter chemistry affects SOM chemistry.

The second objective of our work is to develop tools that facilitate parameter estimation and their associated uncertainties in a cross-site Bayesian data assimilation framework. This objective aims constrain key aspects of microbial physiology and interactions with the physicochemical soil environment that are difficult to quantify. Using observations from a recent meta-analysis we generated posterior predictions for conventional and microbial-explicit models, providing a new level of Bayesian statistical rigor to soil biogeochemical model comparisons. Moreover, with relatively few examples of Bayesian analyses of complex ODEs, our contributions open the door to for others to take advantage of these powerful statistical modeling and data analysis tool.

Our third objective is to develop a testbed to compare, evaluate and improve the representation of global-scale soil biogeochemical models. The testbed provides a computationally tractable, numerically consistent framework to begin exploring the effects of different model structures and parameterizations on soil carbon stocks and fluxes. Preliminary results indicate that the three soil models implemented in the testbed adequately represent global soil C stocks, but project divergent soil C trajectories over the 20th century. We contend that accelerated advancements in soil science, ecosystem biogeochemistry and global modeling will be facilitated by developing tools for evaluating structural, forcing and parametric uncertainties in soil biogeochemical models.

Poster #72

Carbon Cycle Dynamics within Oregon's Urban-Suburban-Forested-Agricultural Landscapes: Impacts of Bioenergy from Additional Forest Harvest and Conversion of Non-Food Crops to Poplar

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Land management strategies within urban-suburban, agricultural, and forested landscapes can have significant impacts on local and regional carbon and water cycles thereby contributing or mitigating effects of global climate change. Decision makers' plans for bioenergy production have long-term implications, though lack fundamental understanding of impacts on ecosystems and atmospheric greenhouse gases. We quantify the interactions and feedbacks between proposed actions, ecosystem processes, and changes in climate on local and regional scales. This is particularly important as strategies for limiting CO₂ emissions are often implemented by states.

We assess the combined effects of changes in land-use and land cover (LULC) and climate on the carbon cycle over Oregon, which has a strong population-vegetation-climate gradient. To meet GHG reduction targets, Oregon's last coal power facility was converted to burn forest harvest residues for bioenergy. Our assessment of availability of forest harvest residues shows the supply is neither sufficient nor sustainable. Forest harvest residues combined with forest thinning where fire return intervals are short produce less than half of the energy supply for the first harvest cycle, and the supply from thinning is reduced in subsequent years. Conversion of Willamette Valley non-forage grass-seed cropland to poplar could nearly supplement the remainder needed annually, but this would require fertilization and irrigation. Furthermore, the land-use change from grass crop to poplar is an unfavorable option to landowners because grass seed is a traditional cash crop. Thus, initial estimates show that burning harvest residue and thinned trees in dry areas vulnerable to fire in Oregon would not appear to provide a sustainable supply for even half of the energy needed annually and would fall short of demand within the first 25 years. Importantly, the net effect is a decrease in the net ecosystem carbon balance of Oregon's forest sector.

Terrestrial Ecosystem Science

Next Generation Ecosystem Experiments (NGEE): Arctic

Poster #1

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

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The Next-Generation Ecosystem Experiments (NGEE Arctic) project is a decade-long (2012 to 2022) study that seeks to improve the representation of high-latitude ecosystems in Earth System Models (ESM). We are conducting a coordinated series of model-inspired investigations in permafrost landscapes near Barrow (recently renamed Utqiagvik) and Nome, Alaska. In Phase 1 (2012 to 2014), researchers applied a multi-scale measurement and modeling strategy for watersheds on the North Slope of Alaska. Knowledge gained on topics ranging from hydrology to plant physiology provided process understanding and parameters that are now being incorporated into DOE's Accelerated Climate Model for Energy (ACME). In Phase 2 (2015 to 2018), we have established three field sites on the Seward Peninsula which, compared to our research site on the North Slope, are characterized by transitional ecosystems; warm, discontinuous permafrost; and well-defined watersheds with strong topographic gradients. These new sites expand our capabilities to investigate (1) landscape structure and controls on the storage and flux of carbon, water, and nutrients, (2) edaphic and geochemical mechanisms responsible for variable 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, (4) controls on shrub distribution and associated climate biogeochemical and biophysical feedbacks to climate, and (5) changes in surface and groundwater hydrology. Our vision in Phase 1, and now extended into Phase 2, strengthens the connection between process studies in Arctic ecosystems and high-resolution landscape modeling and scaling strategies. The NGEE Arctic project supports the BER mission to advance a robust predictive understanding of Earth's climate and environmental systems. The research conducted by NGEE Arctic is coordinated with the NASA Arctic-Boreal Vulnerability Experiment (ABOVE). Safety, collaboration, outreach, and a commitment to data management, sharing, and archiving are key underpinnings of our model-inspired research in the Arctic.

Poster #2

Wetter or Drier? Large Uncertainty in Permafrost Hydrology Projections

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With the historic and predicted deepening of the permafrost active layer, there is a large uncertainty in future projections of hydrological conditions across the Arctic. Since the soil hydrologic state exerts a strong influence on the rate and pathway of soil organic matter decomposition into CO₂ or CH₄, there is a strong need to examine and better understand model projections of hydrologic change and how differences in process representation affect projections of wetting and/or drying of permafrost landscapes. This study aims to advance understanding of where, when and why arctic will become wetter or drier. In particular, we compared simulations of 8 permafrost “enabled” land models ran from 1960 to 2299 period and assessed differences in simulated soil moisture (0-20cm layer) and hydrology variables (runoff and evapotranspiration) across the permafrost region. There is a qualitative agreement between most models but projections vary dramatically in magnitude. Climate models project intensification of precipitation across the Arctic domain while land models indicate that runoff and ET will both increase. In general, the water input to the soil (P-E) also increases, but models project a contradictory general long-term drying of the top soil under a high emissions climate scenario. Simulated drying can generally be explained by increases in active layer thickness and permafrost loss resulting in the transport of near-surface moisture to deeper layers and, where permafrost in a grid cell thaws completely, increased subsurface drainage. Variability among simulations is largely attributed to parameterization and structural uncertainty between participating models, particularly the diverse representations of evapotranspiration, water table and soil water storage and transmission. A limited set of results from single forcing experiments suggest that the warming effect in the sensitivity analysis was the principal driver of soil drying while CO₂ and precipitation effects had a small wetting influence. This analysis serves as a baseline to identify key process representation gaps and opportunities to improve representation of permafrost hydrology and associated projections of carbon and energy feedbacks in land models.

Poster #3

Nitrate and Oxyanion Concentrations in Unsaturated High-Topography Polygonal Features: Implications for a More Fertile Arctic

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The extreme sensitivity of the Arctic system to changing climate conditions is amplifying global feedbacks at an alarming rate. Soil moisture content is a major determinant of nutrient-cycling rates in Arctic soils: with increasing drainage network efficiency and the continuing thawing and degradation of permafrost regions, nutrients are becoming more readily available. Nitrate (NO_3^-) is an essential nutrient within the Arctic and has the potential to increase rapidly with hydrologic evolution toward drying conditions. Here, under the auspices of the Next Generation Ecosystem Experiments: Arctic (NGEE) funded by the DOE, we use field geochemistry to characterize the current nitrate content of unsaturated geomorphic features in the polygonal tundra region of the Barrow Environmental Observatory (BEO), where our data suggests a strong correlation between high nitrate concentration and low soil moisture content. Coupling these geochemistry measurements with remote geospatial observations, we calculate the possible ranges of nitrate content within the BEO and assess the impact of possible future drying scenarios on nitrate production. The projected hydrologic evolution of permafrost regions may lead to a significant increase in nitrate production in future years, and assuming that the entirety of the $\sim 1000 \text{ km}^3$ of polygonal terrain that comprises 53% of the Alaskan Arctic Coastal Plain would undergo the same drying evolution and nitrate production as the BEO, this region has the potential to increase nitrate production by several orders of magnitude. This impending nutrient flux directly impacts primary productivity and biogeochemical cycles within the Arctic and has severe implications for future biological communities.

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Poster #4

Diversity of High and Low Arctic Vegetation in Alaska

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The Next-Generation Ecosystem Experiments (NGEE Arctic) is a 10-year project to reduce uncertainty in Earth System Models through developing a predictive understanding of carbon-rich Arctic system processes and feedbacks to climate. In the first two phases of the project, disparate landscapes in the high and low Arctic in Alaska were chosen to represent the two extremes along environmental gradients. The high Arctic landscape near Barrow, Alaska represents a cold, continuous permafrost region on the Coastal Plain of the north slope of the Brooks Range, while in contrast the low Arctic landscape near Nome, Alaska represents a warm, discontinuous permafrost in a mountainous landscape with strong topographic gradients.

The variation in structure and organization of these two landscape extremes allows for the assessment of how predicted warming and permafrost thaw affect above- and belowground plant functional traits, and ultimately what the consequences will be for ecosystem carbon, water, and nutrient fluxes. In order to accurately make this assessment, the vegetation must first be surveyed and described, and the vegetation-environment relationships must be analyzed and understood.

Here, we describe the vegetation at the high and low Arctic field sites. We include 78 vegetation plots in our analysis that were subjectively sampled from homogeneous plant communities from the high (48 plots) and low (30 plots) Arctic field sites. Plant communities were differentiated and vegetation-environment relationships analyzed using cluster analysis and ordination. We compare and contrast species, functional type, and habitat diversity within plant communities, and between sites. We also report on the main environmental gradients that differentiate the observed diversity.

Poster #5

Recent Advances in Fine-Scale Integrated Modeling of Permafrost Systems

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The Advanced Terrestrial Simulator (ATS) is a tool developed primarily for and by NGEE-Arctic to develop fine-scale, process rich models of eco-thermal-hydrological models of permafrost evolution in a variety of landscapes. Critical to this effort is the recognition that model structure and model coupling is not certain – different problems require different physical components, and accurate and efficient solution of those problems may require different coupling strategies. Here we highlight how ATS enables coupling through the Arcos multiphysics framework using two examples of ongoing work critical for NGEE-Arctic. First we show how ATS has been coupled to Amanzi's transport processes, and then to reactions for biogeochemical simulations through the Alquimia interface. This combined capability, which enables the use of PFLOTRAN and other biogeochemical codes, is becoming the go-to NGEE-Arctic fine-scale modeling capability as it allows biogeochemistry experts familiar with developing nutrient cycles in PFLOTRAN to couple their work with ATS's thermal hydrology. Simulations are constrained through data with a study of the Barrow tracer experiment. Next we demonstrate how ATS and Arcos allow experimentation with coupling strategies through ongoing development of ice-wedge thaw subsidence and frost heave simulations. In this example, it is shown how identical processes are coupled in multiple ways to test the importance of tightly coupling deformation with thermal hydrology.

Poster #6

Quantifying Multi-Dimensional Relationships to Estimate Arctic Soil Properties and Ecosystem Functioning at Relevant Scales

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Arctic soils contain large amounts of carbon in permafrost, which could potentially create a positive feedback to warming climate if released during permafrost thaw. Predicting carbon cycling in Arctic requires quantifying tightly coupled surface and subsurface processes. A main challenge has been a lack of means to sense highly heterogeneous surface and subsurface properties in high resolution and over large areas. In this study, we present two new approaches successfully applied in Barrow, AK to co-investigate surface and subsurface properties at intensive site and to use the inferred relationships to constrain estimates at larger scales.

The first approach focused on estimating soil organic matter content using geophysical methods and simulations of hydrological-thermal processes. Using cores extracted from the Barrow site, we first estimated the spatial distribution of soil organic matter density and geochemical properties through sample analysis and X-ray computed tomography. We demonstrate the value of computed tomography and neural network technique to estimate organic matter density and physical/geochemical properties while increasing spatial resolution and coverage. In addition, we developed an approach to assimilate monitoring and soil sample data into a physically-based joint inversion model that incorporates electrical resistivity data to investigate the extremely dynamic nature of hydrological-thermal processes associated with the influence of soil organic matter and annual freeze-thaw events. The developed joint inversion scheme can estimate the vertical distribution of organic matter content and its control over hydrological-thermal behavior.

A second effort focused on investigating tightly-coupled above/belowground ecosystem functioning using a range of ground-based data (e.g., soil temperature, moisture, thaw thickness and carbon fluxes) and measurements from a track-mounted tram carrying a suite of near-surface remote sensing sensors. Joint analysis focused on correlating key subsurface and ecosystem properties with surface properties that can be measured by satellite/airborne remote sensing over a large area. Our results provided several new insights including: (1) soil temperature (at >5 cm depth; critical for permafrost thaw) was decoupled from soil surface temperature and was influenced strongly by soil moisture, (2) NDVI and greenness index were highly correlated with both soil moisture and gross primary productivity.

Poster #7

Characterization and Partitioning of CH₄ and CO₂ Eddy Flux Data Measured Near Utqiagvik, Alaska

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Arctic regions are currently the most vulnerable ecosystems under our changing climate. Since the advancement in Eddy Covariance measurements, the number of sites in these high latitudes measuring greenhouse gases and energy (CO₂, CH₄ and H₂O), is steadily increasing with new sites being established each year. These valuable data are not only important for annual carbon budget calculations, but also vital to the modeling community in improving their predictions on emission rates and trends.

CH₄ flux measurements are not as straightforward as CO₂ measurements where drivers are known, or as predictable or as easily interpretable as CO₂ fluxes. Understanding CH₄ emission patterns are often challenging. Contributing to these challenges is the limited number of ancillary measurements carried out at many sites and the lack of standardized data processing, QA/QC and gap-filling procedures. As CH₄ flux fluctuations are spatially and temporally diverse, and in many cases event-based, a better understanding or interpretation of results is required. An improvement in understanding also increases the reliability of models, predictions and gap-filling methods, as annual greenhouse gas budgets rely on high quality data.

CO₂, CH₄ and energy flux measurements are ongoing at the NGEA Arctic/AmeriFlux US-NGB site, established in 2012 on the Arctic coastal plain near Utqiagvik (formerly known as Barrow), Alaska. The site, characterized as polygon tundra with underlying continuous permafrost, shows a high degree of inter-annual and seasonal variability in CH₄ fluxes. In order to interpret this variability, we apply a variety of models, such as footprint characterization, generalized additive models, as well as artificial neural networks, in an attempt to decipher these diverse fluxes, patterns and events.

Poster #8

Soil Property Comparisons from the Seward Peninsula

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The Next-Generation Ecosystem Experiments in the Arctic (NGEE-Arctic) project in Phase 2 has added new field sites, including tundra sites with discontinuous permafrost on the Alaskan Seward Peninsula that complement ongoing research in Barrow, AK. One site on the Teller Road (near mile marker 27) comprises a watershed with a peat plateau underlain by permafrost at the top of the hillslope, willow shrubs, mosses, lichens and sedges on drier hillslopes, and a saturated, peaty lowland at the base. We sampled soils at eight intensive sites in this watershed during a coordinated campaign in Sept. 2016. The team dug a soil pit at each site, described soil horizons, and collected thermal and hydrological measurements with depth. We also removed samples from the face of the pit for laboratory analyses of water content, total C and N, and metal content. Macrorhizon samplers inserted into wet horizons extracted water that was analyzed for ions and isotopes, reported separately. Finally, screened piezometers were used to collect soil water samples at wet sites, for field analyses of pH and Fe(II) concentration, as well as laboratory gas chromatography, ion chromatography and ICP-MS analyses of dissolved gases, inorganic ions and organic acids. Substantial differences in thaw depth and water content, dissolved Fe(II) and CH₄, organic acids, soil C and pH among sites illustrated the importance of lateral water flow on controlling oxygenation and SOM accumulation through the watershed. Similar measurements from a flat, peaty tundra site with extensive thermokarsts near Council, AK provide an important comparison with Teller peat plateau and Barrow locations for simulating SOM turnover in carbon-rich sites. This comprehensive data set is being curated and deposited into the NGEE-Arctic Data Portal (DOI:10.5440/1342956) to parameterize initial models of the sites and facilitate planning future fieldwork.

Poster #9

Constraining Arctic Models with Disparate Datasets to Enhance Physical Process Understanding

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The NGEE-Arctic project is collecting a wide array of data in order to characterize and understand Arctic physical processes, including hydrological, thermal, geophysical, geochemical, and biological datasets. The NGEE-Arctic project is improving Arctic physical process knowledge and understanding by constraining models with these disparate datasets. The assimilation of disparate datasets to constrain and test our physical process models provide a synergistic effect improving our Arctic understanding beyond what is possible with a single type of data. For example, we are using hydrological, thermal and geophysical datasets (i.e., temperature, water content, and electrical resistivity tomography (ERT) datasets) to constrain coupled hydrothermal (ATS; <https://github.com/amanzi/ats>) and geophysical (BERT) simulations in a joint inversion to improve our characterization of Arctic soil, water content, salinity, and permafrost structure. This integration of hydrothermal and geophysical data is powerful as the direct observations of temperature and water content provide hard constraints on the inversion, while the ERT surveys provide comprehensive, spatially distributed soft constraints on the inversion. We are also integrating geochemical and hydrothermal data from recent tracer tests in order to improve our understanding of lateral flow in polygonal tundra. Measurements of tracer breakthrough, temperatures, and water content constrain hydrothermal tracer transport simulations using ATS. Ensuring that the ATS simulations are consistent with the hydrological, thermal, and geochemical datasets improves our ability to test hypothesis regarding the relative importance of vertical and horizontal flow in polygonal tundra.

Poster #10

Macrotopographic Controls on Surface Water and Active Layer Chemistry in the Arctic Coastal Plain of Northern Alaska

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Surface water and active layer soil water geochemistry in Arctic environments reflects the chemistry of water sources, water-mineral interactions, soil saturation influence on redox conditions, and biogeochemical cycling of nutrients by plants and microbial communities. Geochemical variation in different types of macrotopography have been reasonably well studied (e.g. polygonal terrain and drained thaw lake basins (DTLBs)), but few comparisons of geochemistry between macroscopic landscape units have been made. Such comparisons are important for assessing hydrologic connectivity in changing Arctic landscapes and in addressing issues of scaling and incorporation of widespread remote sensing data together with sparse geochemical data in climate scale models of hydrology and landscape evolution. In this study, we have focused on characterizing chemical and isotopic signatures of surface water and pore water of perennially saturated active layer soils of different macrotopographic landscape units to assess primary controls on geochemical signatures and to evaluate relative degrees of hydrologic connectivity between units. The location of our study was in and around the Barrow Environmental Observatory (BEO) in Barrow, Alaska, USA. At the BEO, we investigated the geochemistry of three macrotopographic units: 1) relatively high-relief polygonal terrain located between DTLBs, 2) lower lying drainages, and 3) different-aged DTLBs. Active layer chemistry was relatively similar between macrotopographic units, though two locations may reflect additional sources of salinity. This additional source of salinity is possibly associated with cryopegs (partially frozen brine layers that occur in permafrost). At this scale of sampling, it is unlikely that similar chemistry represents strong subsurface hydrologic connectivity within the active layer, but rather similar degrees of water-mineral interaction in active layer soils. Surface water isotope signatures from DTLBs show strong evidence for evaporation, as do drainages connected to DTLBs. Drainages not originating in DTLBs lack strong evaporative signals, suggesting that water isotopes are a useful tool for understanding hydrologic processes and connectivity at the landscape scale. The nearly complete absence of detectable nitrate in the pore water of saturated soils emphasizes the important control soil moisture has on soil redox conditions and biogeochemistry. The effect of thawing permafrost on landscape evolution and soil moisture will have significant feedbacks on nitrate availability (see poster of Arendt et al.).

Poster #11

Modeling Hydrothermal Interaction Within 2D Hillslope

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Arctic hydrological processes impose an important feedback on permafrost thermal conditions. Changes in permafrost hydrology could accelerate its thawing, resulting in a positive effect on permafrost carbon decomposition rates. Therefore, it is important to understand how geomorphic and other landscape processes control permafrost distribution and its properties such as soil saturation, ice content, active layer thickness (ALT) and temperature. The Advanced Terrestrial Simulator (ATS) is a collection of hydro-thermal processes designed to work within a flexibly configured modeling framework. ATS includes the soil physics needed to capture permafrost dynamics, including ice, gas, and liquid water content, multi-layered soil physics, and flow of unfrozen water in the presence of phase change. In this study, we directly address one of the tasks of the NGEE-Arctic project by modeling the effect of climate and environmental drivers on ALT and permafrost thickness and its distribution along the subarctic hillslope. Hillslope flowpaths along with vegetation and soil organic matter distribution, variation in soil depth and mineralogy are important components of the subgrid spatial extent of permafrost. This study explores the ways to improve the quality of the permafrost predictions at the subgrid scale and contribute to the better modeling of the permafrost related processes at the pan-Arctic scale.

Poster #12

The NGEE Arctic Data Archive: Data Sharing Metrics; Manuscript and Dataset Submission Tracking; and Tool Updates and Improvements

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The Next-Generation Ecosystem Experiment (NGEE) Arctic project is composed of an array of researchers and disciplines across multiple national laboratories and universities. Project-generated datasets will improve representation of complex interactions of arctic land surface and subsurface processes in Earth System Models (ESMs). The NGEE Arctic Data Management Team (DMT) at ORNL, with assistance from Data Representatives at each collaborating institution, are charged with collecting, archiving and sharing data within the project, the larger scientific community, and the public. The DMT will present an update on Data Sharing Metrics; Manuscript and Dataset Submission Tracking; and Tool Updates and Improvements.

Data Sharing Metrics: The DMT provides regular updates to the team members, project management and sponsor on data submission and sharing status. The metrics include the number of metadata records available, planned datasets, datasets available to the project or public, and number of data downloads.

Manuscript and Dataset Submission Tracking: The DMT in collaboration with the Project Management Team are tracking the progress of manuscripts together with the associated datasets towards publication. We strive to meet the DOE Office of Science Statement on Digital Data Management requiring data, that support and validate results in a publication, be published at the same time the paper is published. The effort also enhances use of data Digital Object Identifiers (DOIs) and good data citation practices.

Tool Updates and Improvements: The DMT aims to meet the needs of the project team members and scientific community with continuous updates and improvements to the NGEE Arctic data management tools. Similar standards-based, open-source tools are used across multiple projects there by leveraging the DMT expertise across these projects.

Search and Access current data and Submit new data and metadata from the NGEE Arctic home page [ngee-arctic.ornl.gov]. Click the “Data” tab and select either “Search Data” or “Submit Data” on the dropdown menu.

Poster #13

Investigating Bedrock Through Canopy Structure, Organization and Connectivity of an Arctic Watershed

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Improving understanding of Arctic ecosystem functioning and parameterization of process-rich models that simulate feedbacks to a changing climate requires advances in quantifying ecosystem properties, from within the bedrock to the top of the canopy. In Arctic regions having significant elevation gradients and subsurface heterogeneity (bedrock, permafrost, ground ice), quantifying surface and subsurface structure, organization and connectivity of watershed elements is critical yet particularly challenging. In particular, the degree of connectivity or isolation of individual watershed elements will control whether changes in one element will propagate beyond the site of change or remain isolated in space.

In this study, we evaluate linkages between physical properties (incl. soil properties, bedrock depth, permafrost characteristics), hydrological conditions and geomorphic characteristics. This study takes place in a Seward Peninsula Watershed near Nome AK, which is characterized by variable vegetation, significant elevation gradients, extensive bedrock, and discontinuous permafrost. We use a multi-method acquisition strategy to characterize below and above ground properties and their linkages, including point-scale measurements, electrical resistivity tomography, seismic refraction and low-altitude aerial imaging. Data integration and analysis is supported by numerical approaches that simulate dynamic hydrological and thermal processes.

Overall, this study enables the identification of watershed structure and the links between various soil properties (water content, temperature, electrical conductivity), landscape properties (incl. wetness conditions, vegetation, topographic metrics) and the bedrock/permafrost distribution and characteristics in a representative Arctic watershed. For example, results show that permafrost is more present under grassy areas and water saturated soil, while shallow rocky soil is often correlated to regions having no permafrost and increased drainage. These results are consistent with preliminary conceptual models developed for the investigated site. In addition, low-altitude aerial imaging shows promise to extend the landscape organization analysis approach to larger regions in the Arctic. The obtained information about organization and connectivity of the landscape is expected to be useful for improving predictions of Arctic ecosystem feedbacks to climate.

Poster #14

Modeling Shrub Expansion Under Changing Climate Across Arctic Tundra of North America

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Recent changes in species composition and increased shrub abundance in particular has been reported as a result of amplified warming in Arctic tundra. Despite these changes, the driving factors that control recent Arctic shrubification and its future trajectory remain uncertain. Here, we used an ecosystem model, *ecosys*, to mechanistically represent and explain the underlying processes of how plant functional types (PFTs) have changed under climate change in recent decades and will change over the 21st century across the Arctic tundra of North America (NA). Modeled changes in average productivity of shrubs (~35%) over recent decades were corroborated by observed changes (20 – 40%) across different sites of the NA Arctic tundra. Recent and projected warming was modeled to increase thawing of the permafrost, deepen the active layer (~3 cm decade⁻¹), increase nutrient availability, and enhance shrub growth in Arctic tundra. Although spatial heterogeneity and contrasting modeled responses of co-existing Arctic PFTs occur in the predictions, overall increases in shrub productivity was modeled across the tundra, particularly in Alaska and the tundra-boreal ecotone. Increases in graminoids were modeled in the lower central Arctic, while non-vascular plants increased across much of the high-Arctic and declined in the low-Arctic from increased canopy cover of shrubs that limited incoming shortwave radiation for low-lying plants. A particular increase in productivity of fast-growing deciduous vs. slow-growing evergreen shrubs in the warmer low-Arctic was modeled through differences in investment and retention of carbon and nutrients in their leaves under enhanced N mineralization.

Poster #15

Modeled Nitrogen Dynamics in the NGEE-Arctic Polygonal Tundra Landscape at Barrow Alaska

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Most tundra ecosystems are nitrogen (N) limited, yet most large-scale land models of nitrogen dynamics and nitrogen limitations to the carbon cycle have very large uncertainties. Here we apply the *ecosys* model, which has been tested in a wide range of high-latitude sites, to analyze N cycling at the NGEE-Arctic Barrow, AK sites. Our NGEE-Arctic site is dominated by polygonal tundra, and a wide range of measurements has been taken over the past several years in low-centered, high-centered, and transitional polygons. For the modeling analyses, we developed a three-dimensional coupled representation of a polygon and initialized simulations with site observed soil and vegetation properties. *Ecosys* accurately captured observed diurnal and seasonal cycles of net ecosystem carbon exchange, surface energy and water fluxes, thaw depth and soil temperatures, plant biomass, LAI, and soil moisture. Using the well-tested model, we report here on model sensitivity analyses of: (1) the importance of the moss layer in insulating the soil during the summer, and thereby affecting the thaw depth; (2) non-growing season root dynamics and effects on plant N; (3) coupled hydrological and thermal dynamics; and (4) N leaching and gas losses. Implications for long-term ecosystem responses and needed mechanistic treatments in Earth System Model land models are discussed.

Poster #16

Low Temperature Photosynthesis. Light Response Curves from the High Arctic

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Estimates of Gross Primary Productivity (GPP) by terrestrial biosphere models (TBMs) rely on accurate model representation of photosynthesis. In the Arctic model uncertainty over GPP is the dominant driver of an uncertain Arctic carbon cycle. At the heart of many TBMs is the Farquhar, von Caemmerer and Berry (FvCB) model of photosynthesis. In this model CO₂ assimilation is limited by one of two (or in some cases three) processes; carboxylation limited photosynthesis, and electron transport limited photosynthesis. Previously we have shown large model variation in key parameters associated with carboxylation capacity ($V_{c,max}$) and electron transport (J_{max}) and a large discrepancy between model assumptions and measured values of these parameters in Arctic vegetation. Here we extend this work to evaluate current TBM parameterization associated with the empirical relationship between potential electron transport rate and irradiance, which is typically represented in models as a non-rectangular hyperbola. We measured photosynthetic light response curves and the leaf optical properties of six species on the Barrow Environmental Observatory, Barrow, Alaska to determine key parameters associated with the relationship between irradiance and electron transport i.e. leaf absorbance, the convexity term, and apparent quantum yield. Most existing measurements of these parameters have been made within a narrow temperature range (20-30°C) and the scarcity of data collected at low temperature has been highlighted as an important driver of model uncertainty in high latitudes. In addition, model estimates of apparent quantum yield rarely consider real world conditions where low temperature stress may substantially reduce apparent quantum yield in comparison to the theoretical maximum value used by several models. Therefore, to further evaluate the relationship between electron transport and irradiance, and potential low temperature stress we measured light response curves at both 5°C and 15°C.

Poster #17

Plant Traits Across an Arctic Landscape: Above Versus Belowground

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The complex response of ecosystems to climate change is predicted using Earth System Models, many of which utilize the concepts of plant functional types and plant traits to simulate potential fluxes of energy, carbon (C), and nutrients through a given plant community. High-latitude ecosystems are made up of a mosaic of different plant communities, all of which are exposed to warming at a rate double that observed in ecosystems at lower latitudes. Arctic regions are an important component of global Earth System Models due to the large amounts of soil carbon currently stored in permafrost as well their potential for increased plant C sequestration under warmer conditions. Losses of C from thawing and decomposing permafrost may be offset by increased plant productivity, but plant allocation to belowground structures and nutrient acquisition by roots remain a key source of uncertainty in Earth System Models. The relationship between belowground plant traits and environmental conditions is not well understood in high latitude ecosystems, nor are tradeoffs between above- and belowground plant traits. To address these knowledge gaps, the NGEE Arctic project sampled plant species across a variety of different microsites along the Kougarok Hillslope on the Seward Peninsula, Alaska. The vegetation communities sampled included Alder shrubland, willow birch tundra, tussock tundra, dwarf shrub lichen tundra, and non-acidic mountain complex. Within each plant community, aboveground biomass and canopy height were characterized. For each plant species present, specific leaf area, leaf chemistry (%C, %N, %P and $\delta^{15}\text{N}$), and wood density were measured. Belowground fine-root biomass and rooting depth distribution were also determined at the community level. Fine roots from shrubs and graminoids were separated so that specific root area, average diameter, and root chemistry (%C, %N, %P and $\delta^{15}\text{N}$) could be assessed for these contrasting plant functional types. The environmental conditions present across these vegetation types varied greatly and linear mixed effect models were used to determine their relative influence on above- and belowground plant traits. Tradeoffs between above- and belowground plant traits were also examined for both graminoid and shrub plant functional types. The results of this analysis will inform the inclusion of belowground plant traits in Earth System Models and represent a novel contribution of the NGEE Arctic to arctic ecosystem ecology.

Poster #18

Capturing Plant Trait Variation in the Arctic with Remote Sensing

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The inadequate representation of plant traits and trait variation in terrestrial biosphere models (TBMs), including many that underlie the land-surface component of Earth System Models (ESMs), is a key driver of uncertainty in model hindcasts and forecasts of terrestrial carbon, water, and energy cycling and storage. This is particularly relevant for biomes with only sparse observational data availability such as the Arctic and tropics. In the Arctic, uncertainty in the modeling of carbon fluxes has been tied to the lack of key data on plant properties that regulate these processes. What is needed is an approach to bridge the scales between detailed observations of Arctic vegetation in remote locations and the larger, landscape context needed to inform models on parameter variation in relation to climate, soils, topography, perturbations and other edaphic conditions. Remote sensing approaches, particularly spectroscopy, imaging spectroscopy and thermal infrared (TIR), represent powerful observational datasets capable of scaling plant properties and capturing broad-scale spatial and temporal dynamics in many important vegetation properties. In temperate ecosystems we have shown how leaf and imaging spectroscopy (IS) can be used to map a broad range of plant traits across large areas of the continental U.S. and through time. Here we extend these approaches to the high Arctic to evaluate the capacity to scale and map vegetation properties, including biochemical, morphological and physiological leaf traits from the leaf to landscape scales. Our initial focus is on the development of linkages between a range of plant species and remote sensing data within the Barrow Environmental Observatory (BEO), Barrow, Alaska study site. We coupled measurements of leaf chemistry and physiology, including leaf-level gas exchange, with measurements of full range (i.e. 0.3 to 2.5 microns) leaf optical properties (reflectance and transmittance). Our resulting leaf-level spectra-trait models for Arctic vegetation, developed using data collected in the BEO during the 2014-2016 growing seasons, are comparable with existing models from other biomes. Importantly, despite strong variation in leaf morphology and physiology, we are finding a good potential for spectral models to capture trait variation and highlights the possibility to map traits in the high Arctic. Our next steps include the use of Unmanned Aerial Systems (UASs) for very high resolution near surface scaling as well as leveraging the upcoming 2017 NASA ABoVE airborne campaign, which will include flights over Barrow and the Seward Peninsula, to develop algorithms for mapping key traits across broad regions in the Arctic.

Poster #19

Metagenomic Insights into Microbial Communities and Functions across Arctic Polygonal Grounds

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Permafrost soils are one of the world's largest terrestrial carbon storages thus an important focal point for climate change research. With increasing global temperatures, permafrost carbon stores may become available for rapid microbial mineralization and result in increased greenhouse gas (GHG) emissions. In this project, we applied metagenomics to determine the phylogenetic and functional composition of the soil microbiome from polygonal arctic tundra at the Barrow Environmental Observatory (BEO) in relation to the landscape micro-topography and measured GHG emissions. We collected over 200 active layer and permafrost samples along a transect containing high-, flat- and low-centered polygons for three consecutive years. We found a strong correlation between in-situ GHG fluxes and dominant microbial processes. While polygon type was the primary driver of microbial community composition and distribution of metabolic potential, active layer soil and permafrost microbes shared many metabolic functions that are involved in degradation of complex organic carbon compounds. Yet, not all the key metabolic pathways leading to GHG emissions were found across the BEO. For example CH₄ production and iron reduction processes were constrained to wetter low-centered polygons. By contrast, CH₄ oxidation and CO₂ production potential were more prevalent in the drier high- and flat-centered polygons. CH₄ producing and oxidizing Archaea and chemolithoautotrophic bacteria were detected within the same permafrost layers. We hypothesize that nutrients and available carbon in these layers are tightly regulated and recycled. Metagenomics coupled with reconstruction of microbial genomes, detailed measurements of geochemistry and microbial processes aids us in understanding the biogeochemical cycles in Arctic soils and permafrost, and in the future will better inform efforts to resolve uncertainties surrounding ecosystem responses.

Poster #20

Migrating Knowledge Across Scales to Improve Simulation of Arctic Tundra Processes in an Earth System Model

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Based on efforts within the NGEE-Arctic project, we use several watersheds in the Barrow and Seward Peninsula regions of Alaska to demonstrate a modeling approach that connects fine-scale information to coarse-scale simulations. Two major benefits of this approach compared to standard practice with Earth System Models (ESMs) are that multiple sources of fine-scale information can be combined to reduce biases associated with uncertain model boundary conditions, and that reasonable parameterizations of processes known to be important from fine-scale studies can be included in large-scale simulations. As an example of the first type of benefit, we show the relationships among surface weather parameters and between these and surface topography in regions of complex terrain, including microtopography. We demonstrate that joint distributions of fine-scale surface weather forcing can be incorporated in a sophisticated ESM sub-grid scheme to capture variation in the major physical drivers of thermal, hydrological, vegetation and biogeochemical processes over the example watersheds. As an example of the second type of benefit, we relate surface microtopography to the simulated fractional inundated area and lateral connectivity from fine-scale and intermediate-scale simulations, to constrain simulations at the ESM scale. As a second example of improved process representation at large spatial scales, we demonstrate the integration of the 3D reactive transport and thermal-hydrology code PFLOTRAN within the ACME Land Model (ALM, where ACME is the Accelerated Climate Model for Energy). We examine the influence of lateral connectivity on predictions of thermal, hydrologic, and biogeochemical processes through simulation experiments that test the coupled ALM-PFLOTRAN model in 3D and 1D modes. These results are steps toward the NGEE-Arctic Phase 2 goal of improved simulation of pan-Alaska tundra processes associated with climate feedbacks.

Poster #21

Migrating FLOTRAN Reaction Network From NGEE-Arctic into ACME Through a Generic Biogeochemistry Interface

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The Accelerated Climate Modeling for Energy (ACME) program is an ongoing multi-laboratory and multi-institutional collaboration project aiming to build a next-generation Earth system model. “*How do biogeochemical cycles interact with global climate change*” is one of the three high-level science drivers for ACME. Explicit representation of microbial communities and functions in soil biogeochemistry (BGC) processes is a major task in the ACME Land Model (ALM) development. The microbe-enabled BGC module will be implemented in the PFLOTRAN-BGC framework, which has been developed under the NGEE-Arctic project. PFLOTRAN can solve a system of nonlinear partial differential equations describing multi-phase, multi-component and multi-scale 3-D flow and reactive-transport in porous media. We have developed a generic BGC-Interface in ACME to facilitate the migration of NGEE-PLFOTRAN to ACME. The ultimate objective of this interface is to enable flexible and fast development and evaluation of soil BGC modules and their coupling to various thermohydrology and aboveground vegetation modules. The BGC-Interface includes a generic data-structure to pass data between submodels (i.e., vegetation, vegetation and BGC) and allows a selection of multiple instances (e.g., ALM-BGC and PFLOTRAN-BGC for BGC-submodel) for each submodel. We test ALM-PFLOTRAN and compare it to the original ALM and NGEE-PLOTRAN at the Barrow site, AK. Global-scale test of the ALM-PFLOTRAN will also be conducted through this collaboration between ACME and NGEE-Arctic projects.

Poster #22

Snow-Vegetation-Topography-Permafrost Interactions in the Seward Peninsula, Alaska

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Snow is a critical factor in determining hydrologic, thermal, and ecological processes in Arctic landscapes. Snow depth and density, as well as the timing and duration of snow cover directly influence the thermal regime of frozen ground; the amount of spring runoff and water available for replenishing soils, lakes, ponds and wetlands; snow-vegetation-atmosphere energy exchanges; and the timing and duration of subsurface biogeochemical processes. A key goal of the NGEE-Arctic Phase 2 Science Questions 1 and 5 is to understand and predict how spatial heterogeneity in snow interacts with vegetation composition, micro/macro topography and permafrost dynamics as climate warms and precipitation patterns change. NGEE-Arctic researchers are acquiring snow precipitation, depth, density, ground temperature, snow water equivalent (SWE), vegetation composition and structure and permafrost depth data at hilly sites in the Seward Peninsula. These data are collected at a range of spatial and temporal scales using meteorological stations, in-situ gridded and transect-based surveys, ground-based geophysics, and Unmanned Aerial System mapping techniques. NGEE-Arctic modelers are developing statistical and deterministic models to represent the interactions between snow and landscape characteristics to develop a predictive understanding of the coupled evolution of snow, vegetation and permafrost. Data from our preliminary 2016 snow, permafrost and vegetation surveys at the NGEE-Arctic Teller Road site are demonstrating positive correlations between tall vegetation, deeper snow and deeper permafrost. We are applying the ATS model with this data to quantify these relationships for different vegetation height, density and patch size configurations in hilly watersheds. To improve the statistical robustness of our 2017 surveys we use representative analysis to classify the landscape into key ecotype-topotype units to inform and guide our sampling strategy. This approach should allow us to scale our understanding and prediction of snow-landscape interactions, and their evolution with changing climate, from the hillslope to the watershed and larger regions throughout the Pan-Arctic domain.

Poster #23

The Importance of Soil pH in Controlling Organic Carbon Transformations in Arctic Polygon Tundra

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Accurately simulating CO₂ and CH₄ emissions from high latitude soils is critically important for reducing uncertainties in soil carbon-climate feedback predictions. The signature ice-wedge polygons in Arctic tundra have a high level of heterogeneity in soil thermal regime, hydrology and oxygen availability, which limits the application of current land surface models using simple moisture response functions. We synthesized data from incubations of Arctic soils across a wet-to-dry permafrost degradation gradient from low-centered to flat- and high-centered polygons to assess the Community Land Model Carbon Nitrogen (CLM-CN) decomposition cascade with extended anaerobic organic carbon transformations, including fermentation, iron reduction, and methanogenesis reactions. Modification of the Windermere Humic Aqueous Model (WHAM) enabled us to approximately describe the measured soil pH buffering capacity with model simulations. Separate parameterizations of pH response functions for fermentation, iron reduction and methanogenesis improved the simulation of pH evolution, including the initial pH drop due to organic acid accumulation caused by fermentation and then a pH increase due to iron reduction and methanogenesis. Accurate representation of pH evolution also significantly improved CO₂ prediction as the speciation of CO₂ between gas, aqueous and solid (adsorbed) phases were better simulated under varying pH. These results provided critical insights into the process of soil decomposition, and demonstrated the importance of soil pH in controlling biogeochemical reactions in the Arctic.

Terrestrial Ecosystem Science

**Argonne National Laboratory
TES Science Focus Area**

Poster #24

ANL Terrestrial Ecosystem Science SFA: Estimating Arctic Coastal Plain Soil Carbon Stocks Vulnerable to Active Layer Thickening Under Future Climate

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Estimates of the amount and distribution of organic carbon (C) stored in permafrost-region soils are improving but uncertainties remain high, affecting the ability to reliably predict regional C-climate feedbacks. In lowland permafrost soils, much of the organic matter exists in a poorly degraded state and is often weakly associated with soil minerals due to the cold, wet environment and cryoturbation. Thus, climate warming and permafrost thaw are likely to increase active layer thickness and expose relatively labile soil C stocks to enhanced microbial activity and decomposition. Ice wedge polygons are ubiquitous, patterned ground features throughout Arctic coastal plain regions and are large enough (5-30 m across) that a better three-dimensional understanding of the potential vulnerability of their C stocks to regional warming could improve geospatial upscaling of observational data. We investigated the distribution of soil organic C to a depth of 2 meters across three polygon types developed on glaciomarine sediments of the Arctic Coastal Plain of Alaska: flat-centered (FCP), low-centered (LCP), and high-centered (HCP) polygons, with each type replicated 3 times. We found that soil organic C stocks varied across polygon features (troughs versus centers) and differed among polygon types, with HCPs generally having the largest C stocks despite greater ice volumes. Organic horizon and permafrost C stocks increased from FCPs to LCPs to HCPs, in large part due to greater presence of organic horizons in the upper permafrost of LCPs and HCPs. Our detailed polygon profiles also enable estimation of the amount permafrost-stabilized C that could become vulnerable to enhanced decomposition as a result of increases in active layer thickness under future climate as projected by Earth system models. Thus, accounting for polygon-scale (trough to center to trough) and landscape-scale (polygon type) variations could help reduce the uncertainties in observational estimates of potentially vulnerable soil C stocks for areas dominated by ice wedge polygons and contribute benchmarks for constraining model parameters.

Poster #25

Predicting Potential C Mineralization of Tundra Soils Using Spectroscopy Techniques

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The large amounts of organic matter stored in permafrost-region soils are preserved in a relatively undecomposed state by the cold and wet environmental conditions limiting decomposer activity. With pending climate changes and the potential for warming of Arctic soils, there is a need to better understand the amount of the carbon stored in the soils of this region and its potential susceptibility to mineralization. Studies have suggested that soil C:N ratio or other indicators based on the molecular composition of soil organic matter could be good predictors of potential decomposability. In this study, we investigated the capability of diffuse reflectance Fourier-transform mid infrared (DRIFT) spectroscopy to predict the evolution of carbon dioxide (CO₂) produced by Arctic tundra soils during a 60-day laboratory incubations. Soils collected from four tundra sites on the Arctic Coastal Plain and Foothills of the North Slope of Alaska were separated into active-layer organic, active-layer mineral, and upper permafrost and incubated at 1, 4, 8 and 16°C. Carbon dioxide production was measured throughout the incubations. Total soil organic carbon (SOC) and total nitrogen (TN) concentrations, and the DRIFT spectra of the soils were measured. Multivariate partial least squares (PLS) modeling was used to predict cumulative CO₂ production, and the other measurements. DRIFT reliably estimated SOC, TN and the C:N of these soils. Predictive CO₂ production models were good across the different temperatures (1°C, R²=0.77; 4°C, R²=0.82; 8°C, R²=0.82; 16°C, R²=0.80), for soil horizons (Organic, R²=0.70; Mineral, R²=0.79; Permafrost, R²=0.77), and for soils with low C and N concentrations (SOC<10%, R²=0.80; TN<2%, R²=0.76). The number of PLS factors involved varied across different CO₂ production models from 7 to 19. Analysis of the standardized beta coefficients from the PLS models of CO₂ production indicated a small number (8) of influential spectral bands. These bands were associated with clay mineral contents, silicates, and phenolic OH, aliphatic, carboxylic acid, and polysaccharide compounds. These bands were further explored to determine their relative importance in explaining CO₂ production in soils and their indicator capabilities. Our results demonstrate that the DRIFT spectra contained information that can be used for predicting potential decomposability of tundra soils.

Poster #26

Observed and Modeled Spatial Distribution of Uncertainties in Alaskan Soil Carbon Stocks

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Uncertainties in the magnitude and distribution of permafrost soil organic carbon (SOC) stocks are primary contributors to uncertainties in predicted permafrost carbon-climate feedbacks. In this study, we generated 95% prediction intervals of Alaskan SOC stocks (to 1 m depth) by using 585 SOC profile observations, secondary environmental information representing soil-forming factors (climate, topography, land cover types, surficial geology), and geospatial modeling. We compared our results with uncertainties (95% confidence intervals) generated from four CMIP5 equilibrium SOC stock estimates. Our results showed non-stationary environmental controls on SOC stocks across Alaska. Among the investigated variables, land cover had the most heterogeneous control on SOC stocks, whereas elevation exhibited the least heterogeneous control. The magnitude of uncertainties varied spatially. Among observations, spatial prediction of SOC stocks was least uncertain in Coastal Rain Forests (31 – 33 kg C m⁻²) and most uncertain in Bering Tundra ecoregions (28 – 33 kg C m⁻²). The strength of environmental controllers doubled between the most and least uncertain ecoregions. Despite severe underestimation in comparison to observations, CMIP5 models showed the highest confidence in Arctic Tundra (2.5 – 14 kg C m⁻²) and lowest confidence in Intermontane Boreal (2.4 – 27 kg C m⁻²) ecoregions. Among the six major ecoregions considered, the smallest discrepancies between observed and modeled uncertainties were in the Alaska Range Transitions and Intermontane Boreal ecoregions. Our findings can inform efforts towards (1) quantifying uncertainties in SOC observations, (2) representing observed spatial heterogeneity of SOC in large scale models, and (3) improving understanding of large scale SOC dynamics.

Terrestrial Ecosystem Science

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

Poster #33

ORNL's Terrestrial Ecosystem Science – Scientific Focus Area (TES SFA) A 2017 Overview

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Understanding responses of ecosystem carbon (C) cycles to climatic and atmospheric change is the aim of the Terrestrial Ecosystem Science Scientific Focus Area (TES SFA). Our vision is to: **Improved integrative understanding of terrestrial ecosystem processes to advance Earth System predictions through experiment-model-observation synergy**

The TES SFA is guided by the vision that sensitivities, uncertainties and recognized weaknesses of Earth System Model (ESM) predictions inform observations, laboratory and field experiments and the development of ecosystem process modeling. In turn, predictive understanding and findings from the field and laboratory and improved process modeling are incorporated (with the associated uncertainties) into ESMs as explicitly and expeditiously as possible. Overarching science questions are:

1. How will atmospheric and climate change affect the structure and functioning of terrestrial ecosystems at scales from local to global and from decadal to centuries?
2. How will fossil fuel emissions and terrestrial ecosystem processes, mechanisms, interactions and feedbacks control the magnitude and rate of change of atmospheric CO₂ and other greenhouse gases?
3. What are the climate change-induced shifts in terrestrial hydrologic and ecosystem processes that inform assessment of climate change impacts on ecosystem services and society?

The proposed science includes large manipulations, C-Cycle observations, database compilation, and process studies integrated and iterated with modeling activities. The centerpiece of our climate change manipulations is the SPRUCE experiment testing multiple levels of warming at ambient and elevated CO₂ on the C feedbacks from a black spruce–*Sphagnum* ecosystem. **New results in 2017 include new publications on SPRUCE project performance, bog biogeochemistry and deep peat heating results. The root traits task has initiated the FRED data base.** The TES SFA aims to integrate 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. **Cooperatively funded work with researchers at the University of Oklahoma, has led to the development of the Ecological Platform for the Assimilation of Data (Eco-PAD) in the context of a SPRUCE ecological forecasting system.**

Poster #34

Initial Effects of Warming on Water and Solute Yields from a Black Spruce-*Sphagnum* Bog

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The ecology and biogeochemistry of carbon-rich boreal peatland ecosystems is strongly linked to water cycling and transport. Thus, understanding the effects of climate change on peatland hydrology is vital for interpreting biological and biogeochemical responses. The SPRUCE project is a 10-year-long experiment evaluating the response of a northern black spruce-*Sphagnum* bog to elevated temperatures and CO₂ concentrations. Ten enclosures (12-m diameter) were built within the S1 bog in northern Minnesota, and were assigned one of five temperature treatments (+0, +2.25, +4.5, +6.75, and +9°C) replicated at either ambient or elevated (+500 ppm) CO₂ concentrations. Belowground warming was initiated in June 2014, whole-ecosystem warming began in August 2015, and CO₂ addition started in June 2016. Several hydrological processes are measured within each enclosure, including precipitation, transpiration, and near-surface lateral water flux (i.e., outflow). To measure outflow, a subsurface corral was installed around each enclosure, and outflow was allowed to occur naturally through the corral via drains that span the passively draining acrotelm. Water was collected in an externally located basin. The change in water volume in the basin over time was used to estimate outflow, and an autosampler connected to the basin collected flow-weighted water samples for chemistry analyses. These measurements began in summer 2016.

We hypothesized that outflow would decrease under warmer temperatures due to increased evapotranspiration. We also hypothesized that total organic carbon (TOC) concentrations would increase in outflow waters with warming due to accelerated decomposition of surface peats. In 2016, outflow was lower from the warmer enclosures, with the total accumulated flow from the +9°C enclosures approximately a third of the flow from the +0°C enclosures. There were no clear differences in outflow between ambient and elevated CO₂ treatments. TOC concentrations in outflow water were variable across temperature treatments and across the growing season, with a general trend of higher concentrations in water flowing from the +9°C treatments (mean = 72.6 mg/L) than the +0°C treatments (mean = 50.5 mg/L). However, due to the lower outflow from the warmer enclosures, TOC fluxes were lower. These initial results suggest that warming is altering water yields, solutes yields, and pathways of flow in the bog, with potentially cascading effects to carbon cycling and downstream ecosystems. Future work will continue to link changes in water yields and flowpaths with ecological and biogeochemical processes for a more complete understanding of the effects of climate change on bog ecosystems.

Poster #35

Sun-Induced Chlorophyll Fluorescence Auto-Measurement Equipment (FAME) Designed for Use at Eddy Covariance Flux Sites

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The foundation of our biosphere and civilization rests on the food and energy produced by plants using sunlight. Currently there are no readily available instruments capable of continuous and unattended monitoring of plant photosynthesis and physiological stresses in natural environments. To fill this instrument gap, we have therefore developed a prototype field-deployable system for measuring sun-induced chlorophyll fluorescence (SIF) at leaf, individual plant, or canopy-scales: Fluorescence Auto-Measurement Equipment (FAME). Sun-induced chlorophyll fluorescence is emitted from the core of the photosynthetic machinery of plants and is a vital signal of photosynthesis and physiological stress. FAME is based on a number of hardware and software innovations that make it unprecedented in terms of data quality, acquisition rate, versatility, extensibility, and ease of operation. It is a high-performance integration of software and hardware technologies. It is particularly suited for use at eddy flux sites for two reasons. First, FAME permits the measurement of additional environmental variables (e.g., broadband radiation, temperature, humidity etc.)—that are critical to the interpretation of SIF observations—at the same instant as the spectral information. Second, FAME can be easily integrated into existing data acquisition systems. The FAME prototype was successfully deployed at the Missouri Ozark AmeriFlux (MOFLUX) site in September, 2016. We will present the first results of analyses of SIF measurements obtained so far at the MOFLUX site.

Poster #36

Peatland Carbon Cycle Responses to Warming and Elevated CO₂: Early CO₂ and CH₄ Flux Responses and Status of Tree and Shrub Net Primary Production

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Spruce and Peatland Responses Under Climatic and Environmental Change experiment (SPRUCE) is an *in situ* warming by elevated CO₂ manipulation located in a high-carbon, ombrotrophic peatland in northern Minnesota. Methods for warming at large plot scales (12-m diameter) were used. We combined aboveground enclosure walls that create an internally recirculating warm air envelope with soil deep heating to simulate a broad range of future warming treatments of as much as +9 °C. Deep belowground warming was initiated in June 2014 followed by air warming in August 2015. In June 2016, elevated CO₂ atmospheres (eCO₂ at + 500 ppm) were added to half the warming treatments in a regression design.

Post-treatment net surface C flux estimates in the form of CO₂ or CH₄, measured from 1.2 m diameter *in situ* collars associated with both deep and shallow warming were exponentially correlated with whole-ecosystem warming, but the magnitude of the CO₂ flux remained greater than CH₄. The CO₂:CH₄ ratio of evolved gases was reduced. After a lag period of several months, eCO₂ treatments also led to enhanced net CO₂ emissions in September 2016 and enhanced CH₄ emissions just before the onset of winter. The ¹⁴C-signatures of dissolved organic carbon (DOC) and evolved gases suggest C substrate origins reflect recent rather than ancient C sources, and indicate that active microbial respiration at depth is fueled by surface inputs of DOC.

Annual assessments of tree and shrub-level vegetation growth characteristics and aboveground net primary production following a full year of warming treatments (plus 5 months of elevated CO₂ exposures), have not yet shown clear warming or eCO₂ responses above the pretreatment variation present across the plots. Various measures of growth (circumference at dbh, mass accumulation, mass accumulation per live stem, and terrestrial LIDAR based measurements) are being used to track long-term vegetation response.

Plot-level carbon budgets were highly variable across the S1-Bog during the pre-treatment period, and the net C flux ranged from a source of 71 g C m⁻² y⁻¹ to a sink of 34 g C m⁻² y⁻¹ (95% confidence interval). Varying the assumptions regarding the fraction of CO₂ leaving the bog from autotrophic sources (rapidly cycling current year photosynthate), can produce alternate conclusions regarding the sink-source nature of the bog. However, such changes remain within the confidence interval. Future model-data intercomparisons will help resolve the sink-source nature of the bog with warming.

Poster #37

ORNL's TES SFA Data Acquisition, Archiving, And Sharing To Support Publications, Synthesis, And Modeling Tasks

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Data management, archiving, and sharing of data and model products are an integral part of the ORNL TES SFA. The open sharing of all data and results from SFA research and modeling tasks among investigators, the broader scientific community, and the public is critical to advancing the mission of DOE's Program of Terrestrial Ecosystem Science. TES SFA researchers are developing and deploying the data systems, repositories, tools, and integration capabilities needed for the collection, QA, storage, processing, sharing, analysis, and archiving of data and model products.

- These capabilities facilitate model-data integration and provide accessibility to model output and benchmark data for analysis, visualization, and synthesis activities in support of the TES SFA Vision.
- Active data sharing facilitates delivery of SFA products to sponsors, the scientific community, and the public.
- SFA publications may have companion “___: Modeling Archive” and “___: Supporting Data” products to specifically document data integration and modeling efforts.
- Task specific web sites [Fine Root Ecology Database (FRED) (roots.ornl.gov)], access to web-based tools [LeafWeb (leafweb.org)], links to external products (e.g., microbial metagenomes), and data center value-added products (tes-sfa.ornl.gov) enable these interactions.

The SPRUCE experiment (Spruce and Peatland Responses under Climatic and Environmental Change) is a key component of the SFA. SPRUCE has implemented an experimental platform for the long-term testing of the mechanisms controlling the vulnerability of organisms, ecosystems, and ecosystem functions to increases in temperature and exposure to elevated CO₂ treatments within the northern peatland high-carbon ecosystem. If you build it ... data will follow. All data collected at the SPRUCE facility, all results of analyses or synthesis of information, and all model algorithms and codes developed in support of SPRUCE will be submitted to the SPRUCE Data Archive in a timely manner such that data will be available for use by SPRUCE researchers and, following publication, the public through the SPRUCE website (mnspruce.ornl.gov).

This poster highlights ORNL TES SFA tasks including data acquisition system development, data and modeling products, web-based tools, and their availability to project staff and the public.

Poster #38

Implications of Uncertainty in Fossil Fuel Emissions for Terrestrial Ecosystem Modeling

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Given observations of the increase in atmospheric CO₂, estimates of anthropogenic emissions and models of oceanic CO₂ uptake, it is possible to estimate net global CO₂ exchange between the atmosphere and the terrestrial biosphere as the residual of the balanced (closed) global carbon budget. These calculations show that global terrestrial ecosystems are a growing sink for atmospheric CO₂ (averaging 2.12 Gt C y⁻¹ for the period 1959-2015 with a growth rate of 0.03 Gt C y⁻¹ per year) but with considerable year-to-year variability (standard deviation of 1.07 Gt C y⁻¹). Within the uncertainty of the observations, emissions estimates and ocean modeling, this residual calculation is a robust, current best estimate of the global terrestrial sink for CO₂. A task of terrestrial ecosystem science is to explain the trend and variability in this estimate. However, the “[w]ithin the uncertainty” is an important caveat. The uncertainty (2 σ ; 2 standard error; 95% confidence interval) in fossil fuel emissions previously estimated as part of the Oak Ridge National Laboratory TES-SFA is 8.4% (9.9 \pm 0.8 Gt C in 2015). Combined with uncertainty in the other carbon budget components, this results in a 2 σ (95% confidence interval) uncertainty surrounding the global net atmosphere-biosphere CO₂ exchange of \pm 1.6 Gt C y⁻¹. If one ignores the uncertainty, the carbon-budget estimate of net atmosphere-biosphere exchange includes 2 years (1987 and 1998) in which the terrestrial biosphere is a small source of CO₂ to the atmosphere rather than a sink. However, within the 2 σ uncertainty, the terrestrial biosphere may have been a source in 18 of the 57 years. We examine how well global terrestrial biosphere models simulate the trend and interannual variability of the global-budget estimate of the terrestrial sink within the context of this uncertainty (e.g., which models fall within 1 σ or 2 σ of the estimate). The models are generally capable of reproducing the trend in net atmosphere-biosphere exchange, but are less able to capture interannual variability, particularly the magnitude of year-to-year variations. Analysis of the carbon-budget estimate indicates that the trend is primarily associated with the increase in atmospheric CO₂, while interannual variation is related to variations in global land-surface temperature with weaker sinks in warmer years. We examine whether these relationships are reproduced in the models. Their absence might explain weaknesses in model simulations, or models might simulate similar sinks but show different relationships with the apparent drivers of global net atmosphere-biosphere CO₂ exchange. We consider the implications of these comparisons for terrestrial ecosystem science: for both process understanding and representation in models.

Poster #39

Global Parameter Optimization of ALM Using Sparse-Grid Based Surrogates

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Calibration of the ACME Land Model (ALM) is challenging because of its model complexity and large parameter sets. Here we use version 0 of ALM, which is identical in structure to the Community Land Model (CLM 4.5), and has a significant computational burden. Therefore, only a limited number of simulations can be allowed in any attempt to find a near-optimal solution within an affordable time. The goal of this study is to calibrate some of the ALM parameters in order to improve model projection of carbon fluxes. To this end, we propose a computationally efficient global optimization procedure using sparse-grid based surrogates. We first use advanced sparse grid (SG) interpolation to construct a surrogate system of the actual ALM model, and then we calibrate the surrogate model in the optimization process. As the surrogate model is a polynomial whose evaluation is fast, it can be efficiently evaluated with sufficiently large number of times in the optimization, which facilitates the global search. We calibrate eight parameters against five years of annual NEE, TLAI, and LH data from the U.S. Missouri Ozark (US-MOz) tower. The results indicate that an accurate surrogate model can be created for the ALM with a relatively small number of SG points (i.e., ALM simulations), and the application of the optimized parameters leads to a higher predictive capacity than the default parameter values in the ALM for the US-MOz site.

Poster #40

Whole Ecosystem Warming at SPRUCE: Variable Fine-Root Response of Plant Functional Types

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Peatlands are long term reservoirs of carbon (C) and the magnitude and mechanisms of increased C losses from peatlands due to global change are poorly understood. Ephemeral fine roots regulate ecosystem C and nutrient cycling and may be the first to respond to increasing temperatures. Ecosystem warming could increase nutrient cycling rates and total fine-root production. However, relative to aboveground, belowground biomass allocation may decrease with warming. The rooting depth distribution may also respond to changes in water and nutrient availability. Here, we present belowground results from the first year of whole-ecosystem warming at the SPRUCE experiment in Northern Minnesota. SPRUCE (Spruce and Peatland Responses Under Climatic and Environmental change) is a whole ecosystem warming and elevated CO₂ experiment in an ombrotrophic peatland. Ingrowth cores were used to study changes in fine-root chemistry and production along a temperature treatment gradient (0, +2.25, +4.5, +6.75 and +9 °C above ambient), prior to the initiation of elevated CO₂. Initial results from summer 2015 suggest a 3-fold increase in total fine-root production in the +2.25 and +4.5 °C above ambient treatments. However, the +6.75 and +9 °C above ambient treatments show no significant response to warming. The warming response also varied by plant functional type (PFT). Tree fine roots showed a unimodal response to warming with an initial increase in production followed by decreases in the +9 °C plots. Shrub fine-root production remained unchanged except in the +6.75 and +9 °C treatments where production decreased by 50%. Winter (October 2015 to June 2016) fine-root production was also observed in +4.5 °C and higher treatments in all PFTs, suggesting an extended growing season. We will also present results from ongoing analyses on fine-root chemistry to describe changes in belowground C and N allocation after warming. Ecosystem scale experiments are useful to understand ecological and biogeochemical response to climate change and improve predictive power of ecosystem models. Our results highlight non-linear and PFT-specific warming responses that will be useful to parameterize belowground components of peatland models.

Poster #41

Detection and Attribution of the Terrestrial Runoff in the Conterminous United States

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Detection is the process of demonstrating that change has occurred in a defined statistical sense, while attribution is the process of establishing the most likely cause for the detected change with some defined level of statistical confidence. Though the statistical methods of Detection and Attribution (D&A) have been widely used in studies of physical climate variables (e.g., temperature, precipitation and extreme events), their applications on terrestrial ecosystem (e.g., vegetation dynamics, carbon fluxes, and hydrologic cycles) are limited, mainly owing to the lack of long-term observational records and credible model simulations. With the recent availability of long-term runoff observations (1950-2013) and multiple factorial model simulations in continental U.S., we are in a unique position to detect and attribute the multi-year changes of terrestrial runoff from local to continental scales. To disentangle the natural and anthropogenic drivers (e.g., climate change, elevated CO₂ concentration, and land use/land cover change) underlying spatiotemporal changes in runoff, we'll carry out formal and modified D&A analysis using single-factor simulations from fully-coupled Earth system models and offline land surface models, including the latest ACME land model. We hypothesize that in addition to climate change effects, particularly the precipitation, observed runoff trends can also be attributed to individual and combined human effects. The importance of each natural and human drivers, however, is regionally and seasonally dependent.

Poster #42

A Growing and Global Fine-Root Trait Database: Current Coverage and Scientific Applications

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Fine roots are the most active and dynamic portion to the belowground plant system. Fine roots supply plants with nutrients and water critical for growth and represent a significant sink for plant carbohydrates associated with their production and respiration. Despite clear relationships to plant nutrient, water, and carbon cycling, fine roots continue to be one of the most poorly understood components of terrestrial ecosystems. This then strongly limits our ability to model plant growth and forecast future changes in plant productivity. Poor understanding of fine-root systems is primarily due to limited availability of fine-root data as well as difficulties comparing existing root trait data due to inconsistent measurement protocols.

We address the above limitations with the development of the Fine-Root Ecology Database (*FRED*), which serves as a database to house and organize root trait data and facilitate meaningful comparisons of data obtained using comparable methods. *FRED* also captures relevant ancillary data at both the species and site levels to facilitate tests of trait variation across species and climate. *FRED* currently houses over 70,000 root trait observations collected from ~800 data sources covering over 550 root trait and ancillary trait categories. These data include observations in all globally-relevant plant biomes and higher plant types. *FRED* is now publicly available without restriction at <http://roots.ornl.gov> and gives researchers and modelers a powerful tool to assess fine-root traits in a data-rich environment.

We are leveraging *FRED* to initiate two projects that address gaps in our scientific understanding of fine-root processes in the terrestrial biosphere. Our first analysis uses *FRED* data to inform the ACME Land Model (version 0) and test model sensitivities to changes in root related parameters, including novel model conceptualization of root phenology. Overall, changes in fine-root longevity, C/N ratio, root/leaf allocation ratio, and root phenology had the greatest effects on modeled forest growth in the five evergreen, needleleaf forests examined in this exercise. Importantly, capturing interactive effects, and not just main effects, proved to be key in understanding model responses. Our second analysis applies an advanced gap-filling algorithm combined with analysis of trait relationships to assess broad inter-plant and cross biome patterns in belowground plant strategies. Moving forward, we are using *FRED* to highlight trait types and geographic regions that warrant targeted field campaigns to capture data needed to enhance our broad understanding of fine-root traits and the role they play in defining a belowground and whole-plant growth strategy.

Poster #43

Methods and Initial Results for A Model Intercomparison Study in A Northern Peatland

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Whole-ecosystem warming was initiated at the SPRUCE experimental site in northern Minnesota in the summer of 2015. Early *a priori* modeling results indicated large uncertainty in the potential greenhouse gas flux response of this peatland bog ecosystem to warming and elevated CO₂ concentrations depending on the model structural assumptions about nutrient and methane cycling. A new model intercomparison activity was initiated last year to evaluate the performance of wetland models against pre-treatment conditions, to predict carbon fluxes and state variables over the course of the experiment, and to provide guidance to measurement teams about the key processes that are driving the treatment responses and their uncertainties. Here we present a protocol for performing pre-treatment and treatment simulations incorporating uncertainty about future meteorological conditions using standardized model inputs and evaluation metrics. Initial results simulating pre-treatment conditions at SPRUCE from participating modeling teams are also presented. These model results are compared against observations of water table height, vegetation biomass, net primary productivity, and CO₂ and CH₄ flux measurements. A new framework for incorporating model parametric uncertainty is also discussed.

Poster #44

Microbial Responses of Deep Catotelm Peat to *In Situ* Experimental Warming and *Ex Situ* Amendments of Temperature, pH, Nitrogen and Phosphorus

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The Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) experiment is an ecosystem-level manipulation examining how peatland systems respond to increased temperature and CO₂ levels. This experimental manipulations are expected to lead to various changes in ecosystem processes, including microbially mediated biogeochemical cycles that may ultimately alter the overall C balance of these ecosystems. The initial phase of this experiment began over the summer of 2014 by heating deep subsurface peat to +2.25, +4.5, +6.75 and +9.0 °C above ambient plots with a target heating zone of 1.5-2 meters depth. This deep peat heating phase lasted just over 1 year. The response of microbial communities to *in-situ* warming is assessed with qPCR and 16S rRNA amplicon sequencing at eleven discrete depths across the peat profile to a depth of 200 cm. Additionally, metagenomic sequencing was used to characterize microbial metabolic and functional potential on four depths per profile. After one year of deep peat warming, microbial community structure and abundance of bacterial, archaeal, fungal, and methanogenic populations showed strong vertical stratification across the peat depth profile yet no clear response to the temperature treatments. In an effort to identify factors that may be limiting decomposition and microbial community change in deep peat, we conducted a microcosm incubation of deep peat (150-200 cm depth) at 6 and 15 °C to mimic ambient and +9 °C SPRUCE conditions. Additional treatments included elevated pH and the addition of N and P. Microcosms were monitored for CO₂ and CH₄ production, and microbial community dynamics were assessed using qPCR and amplicon sequencing. Increasing temperature resulted in both greater CO₂ and CH₄ production, while elevated pH only resulted in greater CH₄ production. The effects of elevating temperature and pH in combination with N, P, or N+P additions were more variable. Although temperature had little effect on the overall microbial community structure from amplicon 16S rRNA gene sequencing results, there was a shift in the size of bacterial and archaeal populations evident from qPCR assessments. In contrast, N addition (alone and in combination with other variables) as well as pH amendments seemed to have the largest influence on community structure. Collectively both our *in situ* and *ex situ* results suggest that microbial responses in the deep catotelm peat is likely limited by factors other than temperature.

Poster #45

Representing Northern Peatland Hydrology and Biogeochemistry with ALM

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Northern peatlands are likely to be important in future carbon cycle-climate feedbacks due to their large carbon pool and vulnerability to hydrological change. To produce an enhanced ALM_SPRUCE capable of being used for accurate simulations of high-carbon wetland hydrologic and carbon cycle responses for application to plausible future climate conditions. Firstly, we introduce a new configuration of the land model (ALM) of Accelerated Climate model for Energy (ACME), which includes a fully prognostic water table calculation for a vegetated peatland. Secondly, we couple our new hydrology treatment with vertically structured soil organic matter pool, and the addition of components from methane biogeochemistry. Thirdly, we introduce a new PFT for mosses and implement the water content dynamics and physiology of mosses. We inform and test our model based on SPRUCE experiment to get the reasonable results for the seasonal dynamics water table depths, water content dynamics and physiology of mosses, and correct soil carbon profiles. Then, we use our new model structure to test the water cycle and carbon cycle will respond to different warming scenarios.

Poster #46

Synthesis of Four Forest CO₂ Enrichment Experiments Demonstrates a Strong and Sustained Decadal Carbon Sink in Aggrading Temperate Forest Biomass

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Predictive understanding of the future terrestrial carbon sink remains elusive. Forest responses to increasing CO₂ are a large contributor to uncertainty in this understanding. Synthesizing data from the only four, decade long, forest CO₂ enrichment experiments replicated at the forest stand scale, we show a strong, decadal-scale CO₂ sink in aggrading forest biomass. Across ambient and elevated CO₂ treatments, biomass increased over the decade of the experiments in a linear relationship with NPP, i.e. CO₂ did not affect the relationship between biomass increment and cumulative NPP. However, because wood allocation increased as NPP increased, the retention of NPP as biomass was more efficient under increased CO₂. Each forest showed strong within treatment variability in NPP suggesting that the factors governing the retention of NPP as biomass across a range of natural climatic and edaphic variability also govern the retention of CO₂ stimulated NPP.

At the two sites that were not confounded by uncertainty or adaptation to frequent fire disturbance, state-of-the-art ecosystem models under-predicted the biomass stimulation by CO₂. This under-prediction was caused by an under-prediction of both the NPP response to CO₂ and the increase in the wood allocation fraction in response to CO₂. These data, synthesized as part of the Free Air CO₂ Enrichment Model Data Synthesis (FACE-MDS) project, clearly demonstrate a sustained long-term stimulation of forest biomass in response to CO₂ concentrations predicted for the middle of the century. Properly accounting for this CO₂ stimulation of biomass in aggrading forests will be necessary for accurately projecting the future terrestrial carbon sink.

Poster #47

Computational Experiment Design Within A Functional Unit Testing Framework

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A functional unit testing (FUT) framework has been developed to validate key ecosystem processes within Earth System Model by enabling direct comparison with field experimental result. In this poster, we first present the software components of a FUT for the land model within the Accelerated Climate Model for Energy (ACME) and describe the key technologies and functions incorporated in the FUT system implementation. We then demonstrate several computational experiments designed to validate mechanistic ecosystem processes, such as photosynthesis, root dynamics and soil decomposition. At last, we illustrate several new directions for further system improvement, including real time ecosystem process monitoring and experiment data infusion.

Poster #48

Soil Moisture Drives Microbial Controls on Carbon Decomposition in Two Subtropical Forests

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Soil microbes play an important role in soil carbon (C) cycling. However, microbial dynamics influenced by environmental conditions are not adequately understood owing to limited available microbial observations and the lack of model parameterization against data beyond laboratory scale. Here we incorporated soil temperature and moisture responses into the Microbial-ENzyme Decomposition (MEND) model. We parameterized MEND against observed heterotrophic respiration (RH) and microbial biomass C (MBC) from a three-year field experiment in two subtropical forests. The observed variability in RH and MBC were well simulated by MEND. Using long-term site trends, we employed the calibrated model to project the responses of soil organic C (SOC) to gradual changes in litterfall inputs, soil temperature and moisture. We show that, in these subtropical forests, (1) microbes appear to be much more sensitive to decreasing moisture than to increasing temperature or litterfall inputs; (2) temperature increase could have small positive or negative effects on SOC stocks; and (3) increasing labile fraction of litterfall inputs to SOC appears to cause a priming effect and thereby accelerate decomposition. Our results imply that current emphasis in the literature on temperature response of microbial models may be missing the importance of soil moisture.

Poster #49

Ecophysiology at SPRUCE: Impacts of Whole Ecosystem Warming and Elevated CO₂ in A Northern Peatland

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The Spruce and Peatland Responses Under Climatic and Environmental change (SPRUCE) project is a large-scale, long-term experiment investigating the effects of warming and elevated CO₂ on a ombrotrophic bog in Minnesota. Globally, such northern peatlands store an estimated 500 ± 100 Pg C, a disproportionately large amount relative to the land area they cover. SPRUCE is utilizing 10 large (12-m diameter) enclosures to increase air and soil temperatures to a range of targets (+0 °C, +2.25 °C, +4.5 °C, +6.75 °C, +9 °C) under both ambient and elevated (+500 ppm) CO₂ concentrations for 10 years. This poster will focus on the responses of two dominant trees (*Picea mariana* and *Larix laricina*) and two dominant ericaceous shrubs (*Rhododendron groenlandicum* and *Chamaedaphne calyculata*) detailing the methods being used to characterize photosynthesis, respiration and water relations of each species. Results from the first year of treatments indicated that whole ecosystem warming extended the physiologically active season in both spring and fall, increasing the period of active carbon assimilation, but also exposing plants in these treatments to greater risk of damage from extreme cold events. In addition, the drying heat has resulted in increased water stress, indicated by large reductions in predawn water potentials (even in the spring), quicker drying following rain events, and minimum water potentials reached earlier in the day. Initial gas-exchange results suggest some photosynthetic and respiratory acclimation to both temperature and CO₂ treatments, although the degree of acclimation was species-specific. These results indicate the potential for shifts in community composition due to differential biochemical acclimation and stress responses among the dominant species. Such efforts will provide critical data for modeling efforts both at the site scale and more generally for northern peatlands in global dynamic vegetation models.

Poster #50

Carbon and Nitrogen Cycling By Sphagnum in the SPRUCE Experiment

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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, but over time, community shifts, such as replacement of *Sphagnum* by *Polytrichum* in warmer and drier plots could have a significant effect on whole-ecosystem function. Using clear-topped automatic CO₂ chambers, we estimated gross primary productivity (GPP) of the *Sphagnum* community in 2015 to be 424 g C m⁻². This estimate is consistent with an independent estimate of *Sphagnum* community net primary productivity (NPP) in 2015 of 205 g C m⁻², based on measurements of stem elongation, mass per unit stem length, C concentration, and number of stems per unit ground area. In 2016 we employed a new and more direct method of monitoring *Sphagnum* growth inside mesh columns embedded in the bog. NPP in 2016 averaged 117 g C ± 7 g m⁻². There were no effects of the warming or CO₂ treatments on annual NPP, but in ambient CO₂ summer (mid-May to mid-October) *Sphagnum* productivity was well described by a second-order polynomial with peak productivity occurring in the +4.5 °C treatment. Based on an average *Sphagnum* C:N ratio of 34.6, less than 10% of the N needed to support the observed *Sphagnum* production was accounted for in deposition and pore water chemistry. Therefore we investigated the possible N contribution of the *Sphagnum* associated microbiome using 16S rRNA profiling. We found all samples to be dominated by *Alphaproteobacteria* (45-51%) followed by *Acidobacteria* (11-16%) and *Gammaproteobacteria* (8-9%). N₂ fixing diazotroph abundance decreased with increased temperature (6% in ambient control, 3% in ambient + 6 °C) and methanotroph abundance increased with temperature (0.14% in ambient control, 1.3% in ambient + 6 °C respectively). Current experiments are exploring how increased temperature influences diazotroph abundance, N₂-fixation rates and *Sphagnum* net photosynthesis.

Terrestrial Ecosystem Science

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

Poster# 100

Berkeley Lab Terrestrial Ecosystem Science SFA: Belowground Carbon Cycling

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In the Berkeley Lab Terrestrial Ecosystem Science SFA, we conduct basic research on the role of soils in terrestrial biogeochemistry and climate feedbacks. 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 research in the SFA is centered around a coordinated set of model, field, and laboratory experiments to quantify and characterize the roles of different biotic and abiotic processes that influence soil carbon cycling, and how they may shape ecosystem responses to a warming climate. We are conducting two field manipulation experiments, in an annual grassland and a coniferous forest, that involve warming the whole soil profile and adding ¹³C-labelled litter at different soil depths. We are using the experiments to evaluate the influence of soil depth, mineralogy, biota, and microclimate on soil carbon dynamics, and applying these research results and observations to develop and test new model structures and parameters. Currently, global-scale models do not represent the processes that limit microbial utilization of organic substrates, like sorption to minerals, nutrient limitation, and drought. We have developed a soil decomposition model where C cycling is mediated by minerals, nutrients, water, and microbes. We are using experimental data from the deep soil warming and incubations to guide model development in a reactive transport framework (using BeTR; Tang et al. 2013), and integrating this model into the ACME land model (ALMv0.0) to generate process-based hypotheses about the vulnerability of SOC to global change. This poster will present results from the two warming experiments and highlight some recent results from the microbial, mineralogical, biogeochemical, and modeling work being carried out in the SFA. More detail will be given in separate posters on these four areas.

Poster# 101

How Soil Depth Affects Decomposition

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The Lawrence Berkeley National Laboratory Terrestrial Ecosystem Science Scientific Focus Area has performed several experiments tracing isotopically-labeled plant litter as it decomposes into soil organic matter at various soil depths, in a Mediterranean annual grassland and a montane coniferous forest. Here we synthesize the results of those studies to show when and how depth affects decomposition of root litter inputs. We inserted ¹³C-labeled fine-root litter into three depths (15, 50, and 90 cm) of a coniferous forest Alfisol and measured the carbon remaining in particulate (>2 mm), bulk (< 2mm), free light, and mineral soil fractions over 2.5 years. Similarly, we inserted the same litter into the A and B horizons of a grassland Mollisol and measured the carbon remaining over two growing seasons. Finally, we inserted ¹³C- and ¹⁵N-labeled fine root and needle litter in O and A horizons of a coniferous forest Alfisol and measured the C remaining over 10 years. In the coniferous forest soil, depth did not control initial rates of decomposition, with similar rates across 90 cm of depth in the first year and among the O and A horizons in the first 5 years. In contrast, initial decomposition was faster in the B horizon of the grassland due to increased water availability. Over longer periods of time, decomposition slowed at depth in both the grassland and coniferous forest soils. In the A horizon, this was due to the microbial-processed, litter-derived organic matter becoming mineral-associated. In the deeper horizons, decomposition ceased after only a year or two, which could imply that the remaining litter became less accessible or the microbes had become energy or nutrient-limited. In all three experiments, we found surprisingly little downward movement and retention of litter-derived C within the soil profile. A follow-up laboratory study using soil columns confirmed that after 6 months of decomposition and leaching, nitrogen from litter placed at the surface was found throughout the soil profile, while carbon from that litter was not. This is consistent with a large role of preferential flow paths in transport, but appears inconsistent with common soil-model assumptions of homogeneous incremental transport between horizons.

Poster# 102

Otherwise Decomposable Substrates Exhibit Apparent Recalcitrance When Sorbed to Minerals: A Study of Glucose and Organo-Mineral Complexes in Soil

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Soils are a globally important reservoir of soil organic carbon (SOC). It is well established that interactions with minerals, rather than inherent recalcitrance, is a primary mechanism by which otherwise degradable organic matter accumulates and is retained in soils and sediments. However, the bioavailability of organic compounds in mineral-organic-associations (MOA) under varying conditions—including climate conditions—is not well known. To assess the impact of mineral association and warming on decomposition of an easily respirable carbon substrate (glucose), we conducted a series of laboratory incubations at different temperatures with field-collected soils from 10-20 cm, 50-60 cm, and 80-90 cm depth. We added ¹³C-labeled glucose either free or associated with one of two synthetic iron (hydr)oxide phases (goethite and ferrihydrite) differing with respect to crystallinity and to affinity for the glucose sorbate. Our results demonstrate the following: (1) association with Fe (hydr)oxide minerals reduced the decomposition rate of glucose by more than 99.5% relative to glucose added directly to soil; (2) although total (native soil) respiration was much lower in the deeper soils, when normalized by total C the respiration rates did not differ significantly, implying that total carbon availability limits respiration at depth; (3) application of free glucose suppressed respiration of native carbon at 10-20 cm, but enhanced it in the deeper soils; (4) temperature sensitivity of total (native) respiration was greater in the deep soils than in shallow soils; and (5) respiration of the organomineral complex (glucose and iron-(hydr)oxide) was less temperature sensitive than was respiration of native carbon.

Poster# 103

Modeling the Response of Soil Carbon Decomposition and Stocks to Warming with a Focus on Minerals and Microbes

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Climate warming may reduce soil organic carbon (SOC) stocks if higher temperatures increase decomposition rates. It is uncertain, however, how vulnerable SOC is to warming, or what processes— abiotic and biotic — determine SOC stocks over long timescales. In this poster, we will present results of the Berkeley Lab Terrestrial Ecosystem Science SFA aimed at improving our ability to predict SOC cycling. Comparing observed SOC stocks along a 4,000 km transect in South America to model predictions of SOC using a sorption isotherm, we found that mineral sorption capacity was the dominant control over steady-state SOC stock, and that mineral-bound C is vulnerable to warming. Further, our model suggests that soil can gain or lose C after warming, independent of NPP, depending on assumptions about microbial acclimation and sorption. The type of sorption equation used in soil decomposition models has large implications for SOC stock and its temperature sensitivity. Thus, we compared different model formulations of SOC sorption to mineral surfaces, such as Langmuir, linear, and Freundlich, motivated by the diversity of chemical associations between organic and mineral surfaces.

Biotic interactions such as community-level regulation also affect decomposition rates. We evaluated four archetypal microbial models that range in complexity, finding that insufficient limitations on microbial activity result in unrealistic oscillations and insensitivity of C stocks to plant inputs, diverging from observations. We show that a density-dependent formulation of microbial turnover, motivated by community-level interactions, constrains oscillatory behavior. Comparing model predictions to 24 long-term C-input field manipulations reveals that the density-dependent formulation reproduces soil C responses to long-term C-input changes. C inputs also affect decomposition via effects on microbial nitrogen (N) limitation. Using a metaanalysis of carbon-use efficiency (CUE) observations to constrain the modeled effect of N limitation on decomposition, we found that modeled CUE declined with microbial N limitation due to C-overflow and -acquisition strategies that favor N immobilization. Further, competition between two or more microbial populations for N affected the apparent CUE of the modeled community. These model-development activities are part of ongoing efforts to scale abiotic and biotic controls on soil decomposition for inclusion in earth system models. LBNL

Poster# 104

Impact of Warming on Microbiology and Carbon Cycling in Deep Soils.

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Subsoil horizons contain more than half of global soil organic C stocks. While bulk C turnover at depth is slower than it is at the surface, the vulnerability of deep soil C under future climate scenarios is not well understood. In this project of the SFA, we aim to understand how long term warming affects microbial community composition and functioning, with a focus on decomposition of soil organic carbon (SOC) in deep soils. Microorganisms are responsible for both decomposition and formation of SOC. Changes in microbial community composition, functional diversity, activity, and physiology can determine how soil warming will alter soil carbon and nutrient cycling.

The SFA has established two soil warming experiments: At the Blodgett Forest Research Station, a coniferous forest located in the Sierra Nevada foothills and at the Hopland Research and Extension Center, an annual grassland. The treatment warms the whole profile +4°C above ambient while maintaining the natural temperature depth gradient. Samples across the soil profile were collected prior to and during warming for evaluating the effect on microbial community composition (16S rRNA and ITS gene sequencing) and microbial decomposition potential was assessed via extracellular enzyme activity measurements. To assess whether changes in microbial carbon use efficiency (CUE) occurred in response to warming, we carried out lab incubations with ¹³C isotopologues of glucose and pyruvate. At both sites the activity of all enzymes declined with depth. However, at each site microbial biomass and enzyme activities increased due to warming (at all depths), consistent with the observation that soil from warmed plots had 2-3 fold higher respiration of the ¹³C-labeled substrates. Microbial composition and diversity differed significantly across sites and depths, with bacteria hypothesized to have oligotrophic, and more efficient, growth strategies consistently increasing with depth. Under warming, some of these bacterial groups, such as the Verrucomicrobia in surface soils and Acidobacteria in deeper soils became more abundant. Fungal populations did not appear to be significantly affected by warming. After two years of warming (i.e., in short term incubations using soils collected two years after warming began), respiration of ¹³C-labeled substrates increased 2-3 fold. Microbial CUE varied by depth and time; the initial decrease in the first six months period was followed by increase during the course of warming. Contrary to our expectations based on prior warming studies, microbial CUE increased in response to warming in both surface and deep soils. Our results show that in both forest and grassland soils, warming induced increases in microbial biomass at all depths, coinciding with greater extracellular enzyme activity that may generate positive feedbacks with SOM decomposition and respiration; however increases in CUE due to selection for organisms with more efficient growth strategies may off-set some of this potential for positive feedback.

Terrestrial Ecosystem Science

**Pacific Northwest National Laboratory
Soil Biogeochemistry Study**

Poster# 105

Pore- to Core-Scale Research to Inform Ecosystem-Scale Soil C Biogeochemistry: Drought and Wetting Events Alter Soil Carbon Dynamics

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Droughts and other extreme precipitation events are predicted to increase in intensity, duration and geographic coverage, with uncertain implications for terrestrial carbon (C) persistence and vulnerability. Soil models have difficulty reproducing C dynamics after such extreme events, perhaps due to an inadequate representation of how processes in the interconnected soil pore network interact with abiotic drivers, such as antecedent drought conditions, to alter larger-scale C fluxes. Soil wetting from above (precipitation) results in a characteristically different pattern of pore-filling than wetting from below (groundwater). Building on our previous research demonstrating that different chemical classes of C are associated with particular soil pore size domains, we hypothesized that this differential pore-scale wetting will affect soil C mineralization, especially when soils are rewet following drought conditions. Our findings suggest that classic studies that used field-moist soils under static moisture conditions—upon which predictive models have been parameterized—may constitute a “best-case” scenario. Wetting direction interacted with antecedent drought and physical protection of C to significantly increase the rate and quantities of gaseous C emissions from the soil. These losses may be attributed to broader conditions of bioavailability, driven by C solubilization and transport to microbially colonized and metabolically favorable locations with the soil matrix. Models, which are increasingly microbially-oriented, should treat soil moisture within a three-dimensional framework emphasizing hydrologic conduits for substrate and resource diffusion. As droughts and shifts in precipitation patterns increase, understanding how these events interact at a variety of scales is essential in order to improve predictions of the C sink/source capability of global soils.

Poster# 106

Pore- to Core-Scale Research to Inform Ecosystem-Scale Soil C Biogeochemistry: Effects of Soil Moisture on Heterotrophic Respiration Across Spatial Scales

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Soils store an enormous amount of organic carbon (SOC), but the potential lability of this carbon pool is poorly understood. In particular, our understanding of how soil heterotrophic respiration (R_H) interacts with soil water content (θ) is limited both by sparse observations and the empirical model formulations used by most earth system models. Improved mechanistic models linked to microbial population distribution, substrate access, and hydraulic conductivity are urgently needed. We derived and tested a novel, three-parameter moisture function (f) developed from pore-scale process knowledge and simulations. We tested f against a wide range of published data for different soils, and found that it predicted diverse R_H - θ relationships well. This function represents a mechanistic foundation for understanding how underlying processes affect the R_H - θ relationship in different soils, directly linking the pore-scale mechanisms with macroscale observations. Working at larger spatial scales, we also examined the question of whether changes in global R_H are driving already-observed changes increases in total soil respiration (R_S). Using an expanded global soil respiration database, we document increases in observed R_H : R_S ratios over time, frequently associated with precipitation changes; show this is consistent with multiple complementary lines of evidence; and finds that these trends are robust to sampling variability with respect to ecosystem type, disturbance, measurement methodology, and climate normals. Taken together, these cross-scale model and data analyses emphasize the importance of mechanistic models tightly linked with broad-scale data syntheses.

Terrestrial Ecosystem Science

Next Generation Ecosystem Experiments (NGEE): Tropics

Poster# 75

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. Next Generation Ecosystem Experiments (NGEE)–Tropics is a ten-year, pantropical, collaborative research project aimed at improving Earth system model representation of tropical forest ecosystem responses to global changes. The overarching goal of NGEE–Tropics is to determine how tropical forest carbon balance and climate system feedbacks will respond to changing environmental drivers over the 21st Century.

To accomplish this goal, NGEE–Tropics will develop a transformational, process-rich model framework where the evolution and feedbacks of tropical forests to a changing climate are modeled at the scale of a next generation ESM grid cell. Research in Phase 1 will develop 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. Model development and measurement activities will be integrated at pilot study field sites. A data synthesis and management framework will be developed to build and provide data products via a community portal. Phase 1 will provide a foundation for research on pantropical forest interactions with climate for NGEE–Tropics Phases 2 and 3.

Poster# 76

Software Developments in the Functionally Assembled Terrestrial Ecosystem Simulator (FATES)

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The Functionally Assembled Terrestrial Ecosystem Simulator (FATES) represents processes related to the demographics and dynamics of aboveground vegetation, often in an earth systems model context. It serves as a focal component of the Model-Experiment (MODEX) approach to the Next Generation Ecosystem Experiments (NGEE)–Tropics. This is a tool to probe our understanding of the terrestrial carbon sink and forest response to a changing climate and human activities. It is co-developed with scientific measurement experiments that are designed specifically to improve our understanding of model process and parameterization. FATES is a successor of the Ecosystem Demography model, and had originally been coupled with the Community Land Model, ie CLM-ED. The work presented here describes refactoring to isolate the FATES code into a standalone module and create a well documented public API. The API allows FATES to be incorporated into a range of host models, specifically targeting the Accelerated Climate Model for Energy (ACME). Further, the work presented here also covers efforts to make the FATES model robust, verifiable and integrated with benchmarking and workflow tools such as the Predictive Ecosystem Analyzer (PEcAn).

Poster# 77

NGEE Tropics Data Collection and Management

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The NGEЕ Tropics Data Team works closely with the project's scientists to 1) efficiently generate and synthesize ecological, hydrological, and meteorological datasets from tropical forests in Central and South America for scientific analysis and model parameterization / benchmarking, 2) host all project data, in a community accessible archive and release those data to the public after 18 months in compliance with the NGEЕ Tropics Data Policy, 3) standardize data and metadata collection, and 4) create priority data products such as meteorological model drivers, perform Quality Assurance/Quality Control (QA/QC) of field based observations, and synthesize sapflux measurements collected across 9 field sites collected during the 2015-2016 El Niño.

Project data are archived using the NGEЕ Tropics Archive tool, which allows users to upload and search data packages. Currently, NGEЕ Tropics team members and collaborators can create, save, edit, and submit draft data packages of any content and provide essential metadata in a user-friendly form. Once curated, the data package's metadata are visible to all users of the Archive tool. Three levels of access are enabled for the data files in the package – Public, NGEЕ-Tropics and Private. The system enables users to obtain a NGEЕ Tropics custom DOI for their data. Currently there are a total of 21 records in the NGEЕ Tropics Archive, with 4 being publicly shared (with DOIs).

The metadata reporting framework, implemented in conjunction with the NGEЕ Tropics Archive enables cross-site and cross-method comparison, data interpretability, and QA/QC. The metadata reporting framework leverages several existing metadata protocols, such as AmeriFlux and Smithsonian Tropical Research Institute. It has been implemented for sensor-based observations, such as sapflux, leaf surface temperature, and soil water content. The framework consists of templates that define a multi-scale measurement position hierarchy, descriptions of measurement settings, and details about data collection and data file organization. The framework also enables data providers to define data-access permission settings, provenance, and referencing to enable appropriate data usage, citation, and attribution. Six core NGEЕ Tropics field sites in Brazil, Panama, and Puerto Rico, as well as collaborators, have used the metadata templates to submit data packages to the NGEЕ Tropics Archive.

The NGEЕ-Tropics Archive and metadata reporting templates enable long-term preservation of project data, enforce compliance with the NGEЕ Tropics data policy, and also provide the organization and standardization needed to transform diverse and complex ecohydrological data into scientific understanding.

Poster# 78

Synthesis of Tropical Forest Sapflow Responses to the 2015-2016 ENSO Event: Insights into Key Plant Traits and Mechanisms

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Tropical forest responses to moisture remain poorly understood, in part because of the large diversity of plant hydraulic traits found therein. Changing moisture regimes, such as more frequent drought events, are expected to interact with these diverse hydraulic traits and other requirements of tropical trees in complex ways, making prediction of ecosystem-scale responses and community compositional trajectories difficult. A first step towards discerning such responses is in the analysis of how plant hydraulic and edaphic conditions control trajectories of individual trees' water use over pre-drought, drought, and recovery periods. We took advantage of the 2015-2016 ENSO event, which induced drought over much of the tropics, to collect sap flow data from more than 50 trees across multiple sites situated along a precipitation gradient, enabling us to determine a range of responses to decreasing water resources. Where available, via measurements on conspecific individuals or species-mean values in trait databases, plant hydraulic traits were associated with individual sap flux trajectories, in addition to site-specific soil properties and climate. We found a large heterogeneity of sap flow responses during the ENSO within and among study regions. The diversity of strategies to deal with drought stress was partially explained by species functional traits, background climate and intensity of soil water depletion during the ENSO. Preliminary simulations of drought responses using the Community Land Model coupled to the hydraulically-enabled Functionally Assembled Terrestrial Ecosystem Simulator (CLM-FATES-Hydro) are used to demonstrate multiple mechanisms, both edaphic- and plant trait-related, responsible for the divergence in observed sap flow responses, as well as highlight critical field measurements needed to discern among these mechanisms.

Poster# 79

Improving Plant Functional Types in Earth System Models: Pan-Tropical Analysis of Tree Survival across Environmental Gradients

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Terrestrial carbon cycling is a function of the growth and survival of trees. Current model representations of tree growth and survival at a global scale rely on coarse plant functional traits that are parameterized very generally. In view of the large biodiversity in the tropical forests, it is important that we account for the functional diversity in order to better predict tropical forest responses to future climate changes. Several next generation Earth System Models are moving towards a size-structured, trait-based approach to modelling vegetation globally, but the challenge of which and how many traits are necessary to capture forest complexity while retaining computationally efficient models remains critical. Additionally, the challenge of collecting sufficient trait data to describe the vast species richness of tropical forests is enormous and typically we do not have species level traits available. We propose a more fundamental approach to these problems by characterizing forests by their patterns of size-dependent survival. We expect our approach to distill real-world dynamics into a reasonable number of functional types for efficient modeling.

Using 14 large-area tropical forest plots that span geographic, edaphic and climatic gradients, we model tree survival as a function of tree size for almost two thousand species. We found four categories of size-dependent survival functions emerge. This indicates fundamental survival strategies at play across diverse forests providing reasonable constraint to the range of plant functional types. We mapped common plant traits onto these survival strategies and found little evidence for between site variation in wood density, seed mass and leaf mass per area. We related the relative biomass of our survival strategies to long term environmental variables and found that mean annual temperature and cumulative water deficit were strong predictors suggesting predictability of shifts in community composition with changing climate. We compare size-structured survival in DOE's FATES model with our observational results and offer potential improvements in how mortality is represented in this dynamic global vegetation model to greatly reduce uncertainty about carbon cycling.

Poster# 80

Seasonal Fluxes in the Contribution of Stored Water to the Transpiration Stream: Testing a Hydraulic Transport Model Against Measurements

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In vascular plants, transpiration (E) is often limited by the rate at which water can be transported from the soil to the leaf. Declines in water pressure in soil and plant tissue reduce the transport rate, while water stored within plant tissues modulates plant water pressure, and therefore augments E . Stored water has been estimated to contribute 5–35% of E , depending on plant size, environmental conditions, and plant hydraulic traits. Because E is linked to carbon uptake and photosynthesis, as well as plant growth and mortality, Earth System Model (ESM) development has focused on integration with models of plant hydraulic transport and water storage. However, of these hydraulically-enabled ESMs, none has been tested against measurements in tropical forest trees, where seasonality of water availability combined with high trait diversity may produce divergent patterns of stored water use and E . We measured E and stored water use for five tree species during wet and dry seasons in a seasonally dry tropical forest in Panama. We also measured parameters required for hydraulic transport models to estimate E and stored water use, including water pressure and hydraulic traits. With these datasets, we tested the ability of the hydraulically-enabled Functionally Assembled Terrestrial Ecosystem Simulator coupled to the Community Land Model (FATES-CLM) to predict E , stored water use, and midday leaf and stem water pressure for a set of trees with diverse traits and under varying environmental conditions. Initial analyses of the measurements show that the contribution of stored water to E varied among individuals and seasons, ranging ~5–20% of daily E . Likewise, the direction and magnitude of seasonal change in daily E varied among trees. These observations will be tested against model outputs with a particular focus capturing how variation in hydraulic traits leads to variation in E and stored water use.

Poster# 81

To What Extent Can Variability of Tropical Vegetation Growth Be Predicted Using Sea Surface Temperatures?

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Sea surface temperature (SST) largely controls spatiotemporal changes in global precipitation, temperature and radiation, modulating terrestrial ecosystem productions, especially in the tropical region, where the most productive biome on earth exists. The lag in response of terrestrial ecosystem to SST variations from different ocean regions, however, offers a unique opportunity to investigate the predictability of tropical vegetation growth with SST even several months in advance. Using latest fine spatial resolution remote-sensing vegetation indexes, observation-based GPP products, and SST indexes from different ocean basins (e.g., the Pacific, Atlantic, and Indian) for the period 2000–2013, we thus aim to address the following scientific questions. How does ecosystem production react to SST dynamics on seasonal to intra-seasonal time scales? Which SST index or combination of SST indexes has the most pronounced influences on the tropical ecosystem dynamics? How many months do SST index lead the onset of vegetative responses? How well does the empirical model based on the understanding of vegetation responses to SST can predict vegetation dynamics? We will examine the predictability of vegetation dynamics in response to SST based their correlations and regressions with SST for selected historical period (e.g., 2000-2012). We will establish an empirical model with optimal parameters for the hindcast prediction. We will then validate the stastical model against independent observations that were not involved in the model construction (e.g., the same observations for year 2013 or different observational data). We will finally evaluate the reliability of the statistics-based model at extracting key oceanic impacts on tropical terrestrial ecosystem production using dynamic experiments of ACME driven by observed SST.

Poster# 82

Advancing the Mechanistic Understanding and Model Representation of Photosynthesis and Transpiration Processes of Tropical Evergreen Forests

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Accurate representation of tropical evergreen forest photosynthesis and stomatal conductance in Terrestrial Biosphere Models (TBMs) is a critical component of improving the ability of TBMs to capture the huge fluxes of carbon and water exchanged by tropical evergreen forests. Here we have addressed two key questions; (1) how can TBMs represent tropical evergreen forest photosynthetic seasonality and (2) what existing formulations are best suited to represent tropical evergreen forest stomatal conductance?

Photosynthetic seasonality in tropical evergreen forests results in an annual seasonal fluctuation in CO₂ assimilation of about 6.25 Pg CO₂ over the Amazon basin. We explored alternative options for the incorporation of this quantitatively important seasonality in TBMs that employ the Farquhar, von Caemmerer & Berry (FvCB) representation of CO₂ assimilation. We developed a two-fraction leaf (sun and shade), two-layer canopy (upper and lower) photosynthesis model to evaluate how three components of phenology, i.e. leaf quantity, quality, and within-canopy variation in leaf longevity affect photosynthetic seasonality. This approach identified a parsimonious formulation for representing tropical evergreen forest photosynthetic seasonality in TBMs and highlighted the importance of leaf quality and its within-canopy variation for accurate representation of canopy-scale photosynthetic seasonality.

A critical component of TBM representation of carbon and water fluxes is the formulation used to determine stomatal conductance. Using a large data set we collected of diurnal measurements of CO₂ assimilation and stomatal conductance, we assessed the ability of three leaf level models to simulate observed stomatal conductance and evaluated the importance of accounting for variation between species. Our results showed that stomatal conductance models that accounted for vapor pressure deficit (VPD) performed better than those that did not include VPD in their formulation. We also found that including species specific parameterization of stomatal slope – a key model input – improved model skill. Interestingly, our analysis showed that stomatal slope could be approximated by a commonly measured leaf trait -leaf mass per area and soil moisture content.

Poster# 83

Prediction of Individual Tree Mortality in Tropical Forests Using Inexpensive Field Methods

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Individual mortality is a fundamental component of the life-history of tree species. Variation in mortality rates drives forest structure and dynamics, floristic composition, and carbon and nutrient cycles. A much better understanding of what determines the spatial and temporal variation in mortality rates is required to more accurately predict the future of the global carbon sink. As part of the Next Generation Ecosystem Experiment (NGEE) Tropics, we developed a protocol to monitor annual tree and biomass mortality, including an assessment of factors associated with the death of trees that may help in predicting future tree mortality. The protocol includes assessment of mode of death, nature of tree damage (broken, uprooted, standing), estimation of remaining biomass (proportion of remaining trunk and crown), and assessment on other aspects potentially related to the probability of survival (crown illumination, degree of leaning, liana infestation, presence of fungi, wounds, trunk deformities, leaf damage, etc.). The protocol is both space- and size-stratified to ensure detection of habitat and size-related variation in mortality patterns. The protocol is currently being implemented in 10 large-scale plots (16-52 ha) in CTFS-ForestGEO network.

To investigate potential patterns of mortality in one site, we analyzed the impact of crown damage, crown illumination, wood density and prior growth on survival in the Lambir CTFS-ForestGEO plot (Malaysia), using four censuses of ~28,000 trees ≥ 10 cm dbh between 1992 and 2008. We are using structural equation modeling to disentangle causal relationships affecting survival and correlations due to life history trade-offs.

Poster# 84

Tropical Forest Recovery Following Disturbances: A Remote Sensing Approach

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Tropical forests play major roles in the Earth system. By absorbing and storing large amounts of atmospheric CO₂, tropical forests help reduce anthropogenic warming effects. And by exchanging water with the atmosphere, tropical rainforests act as a global center of rainfall. A key component of tropical forest dynamics is tree mortality that affects, among other features, patterns of productivity, biomass, and floristic composition. How disturbed natural forests recover depends upon complex interactions among soil, climate, tree species, etc. However, our current understanding of that recovery is limited due to the scarcity of observational studies. Remote sensing offers a unique means to study post-disturbance recovery. Here we explore this possibility.

Poster# 85

How Does Variation in Rainfall or a Drier Climate Affect Aboveground Biomass and Tree Mortality of a Seasonally Dry Tropical Forest in Panama?

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Tropical forests store more carbon in aboveground biomass (AGB) than any other terrestrial ecosystem on the planet. This carbon is largely stored in trees belonging to a range of plant functional types (PFTs) with different sensitivities to light and water resources. Climate models vary widely in their predictions of how precipitation patterns may change over tropical forests by the end of this century. The implications of how such changes may affect mortality rates and AGB of different PFTs is unclear. Land surface models that include demographic and plant hydrodynamic processes, such as the Ecosystem Demography model (ED2-hydro), are promising tools for resolving this uncertainty. In this study, ED2-hydro was driven with local meteorological drivers reconstructed to represent several of the predicted, yet contrasting, precipitation scenarios. These scenarios included less interannual variation, longer dry seasons, recurring El Niño related droughts, drier dry seasons, and drier wet seasons. ED2-hydro allows for dynamic competition between four PFTs—early- versus late-successional groups subdivided into drought-tolerant versus -intolerant groups—to occur along water and light resource gradients. ED2-hydro predicts that plant available soil water (PAW) will vary considerably between the different precipitation scenarios. In the simulations, PAW is regulated by both the mean and variation in precipitation, but can be buffered by increased rooting depth. Accordingly, ED2-hydro predicts that changes in the mean or variation of PAW will differentially alter the mortality rates of the four simulated PFTs, which in turn will lead to different AGB outcomes of each. Less variable precipitation tends to reduced AGB of drought tolerant PFTs, while a significant reduction in mean precipitation or greater variation caused by more extreme and frequent droughts tends to reduce AGB of drought intolerant PFTs. ED2-hydro predicts that total ecosystem AGB, however, will only be marginally altered by most of the precipitation scenarios. The only precipitation scenario that leads to a significant reduction in AGB by the end of this century is an intensification of the dry season. Model predictions are consistent with the intermediate disturbance hypothesis where some variation in precipitation, which includes El Niño related droughts and anomalously wet years, is important for promoting functional diversity; but, less variation, a significant reduction in the mean, or more frequent and intense droughts may be destabilizing to functional diversity.

Poster# 86

Impacts of Forest Degradation on Water, Energy, and Carbon Budgets in Amazon Forest

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Forest degradation as a result of logging, fire, and fragmentation not only alters carbon stocks and fluxes in tropical forests, but also impacts physical land-surface properties such as albedo and roughness length that impact boundary layer dynamics and the exchanges of water and energy fluxes between the land and atmosphere. Such impacts are poorly quantified to date due to difficulties in accessing and maintaining observational infrastructures, and the lack of proper modeling tools for capturing the interactions among biophysical properties, ecosystem demography, and biogeochemical cycling in tropical forests.

To address these limitations, we developed and applied two land surface/ecosystem models capable of simulating such interactions: the Ecosystem Demography Model (ED-2) and the Functional Assembled Terrestrial Ecosystem Simulator (FATES) coupled to the Community Land Model. To evaluate the models' ability to represent short-term impacts of forest degradation, we parameterized both models to reproduce the selective logging experiment carried out at the Tapajos National Forest in Brazil. Both models were spun up until they reached steady state, and simulations with and without logging were compared with the eddy covariance flux towers located at the logged and intact sites. The sensitivity of simulated water, energy, and carbon fluxes to key parameters associated with soil properties and plant functional traits were quantified by perturbing the parameters within their documented ranges from literature. The sensitivity to initial conditions is also assessed by initializing the models from forest inventory data.

Our results suggest that both models were able to reproduce water and carbon fluxes in intact forests, although sensible heat fluxes were overestimated, even using the best parameter set within the ensemble. The effect of degradation levels on fluxes, including conventional and reduced impact logging, were assessed by specifying different disturbance parameters in the models (e.g., size-dependent mortality rates associated with timber harvest, collateral damage, and mechanical damage for infrastructure construction). The model projections suggest that even though most degraded forests rapidly recover water and energy fluxes compared with old-growth forests, the recovery times for carbon stocks, forest structure and composition are much longer. In addition, the recovery trajectories are highly dependent on choices of parameter values.

Our study highlights the advantages of an Earth system modeling approach, constrained by observations, to quantify the complex interactions among forest degradation, ecosystem recovery, climate, and environmental factors. This pilot study provides a roadmap to improve the representation of forest degradation in FATES.

Poster# 87

Recovery Time of Carbon, Structure and Functioning of Degraded Forests in the Amazon

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Land use and land cover changes have a major impact in the global carbon cycle, and the impact of these changes in tropical forests are of particular interest because they store about a quarter of total terrestrial carbon stocks. Deforestation in the Amazon, the largest contiguous tropical forest, has declined over the last decade, yet forest degradation from logging, fire, and fragmentation continues to impact forest carbon stocks and fluxes. The magnitude of this impact remains uncertain, and observation-based studies are often limited by short time periods or small study areas.

To better understand the long-term impact of forest degradation and recovery, we are developing a framework to simulate the impact of forest degradation and quantify the typical recovery time for biophysical properties, carbon stocks, and forest structure. This framework integrates forest inventory plots and airborne lidar measurements in intact and degraded forests (conventional and reduced-impact logging, logging and burning, and multiple burns) in the Ecosystem Demography Model (ED-2), a cohort- and process-based ecosystem model that represents changes in carbon stocks and forest structure and functional groups. Based on the model projections initialized with contemporary forest structure and composition, most degraded forests rapidly recover (30 years) water and energy fluxes compared with old-growth forests, even at sites that were affected by multiple fires. However, degraded forests maintained lower carbon stocks and distinct forest structure even after 100 years without further disturbances, because of persistent differences in forest structure and composition. Simulations that included fire suggest that the most degraded forests would take much longer to recover biomass typical of old-growth forests because open canopies and drier microclimates in degraded forests increased the frequency and intensity of recurrent fires. Our study highlights that recovery of degraded forests may act as an important carbon sink over multidecadal to century-long time periods, given fire exclusion to sustain forest recovery. Preliminary results on the recovery of degraded forests following selective logging with different degradation levels using another cohort-based model, the Functional Assembled Terrestrial Ecosystem Simulator (FATES) coupled to the Community Land Model, will also be discussed.

Poster# 88

Assessing Development Needs in Earth System Models by Hydrological Modeling in the Asu Catchment Using a Hierarchy of Hydrological Models

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Current Earth System Models (ESMs) have limited ability to represent key features of tropical hydrology, such as spatial variability in water flows and water available for plant use. To identify development needs for modeling surface and subsurface hydrology in ESMs, hydrological simulations are performed over the Asu catchment, 80 km northwest of Manaus in the Amazon. Models including the ACME Land Model (ALM), DHSVM, CLM-PAWS, h3D, tRIBS, CLM-ParFlow, CLM-PFLOTTRAN, and Amanzi/ATS, with soil hydrology representation from one dimensional to three-dimensional, respectively, are applied to simulate hydrologic variability. 3D model results showed the flow system at the catchment is topography controlled local flows which have the greatest interchange with surface water. Simulation differences were found across models in terms of the temporal and spatial variability of ET, soil moisture, groundwater table and runoff. Comparison of one to three-dimensional models provides an opportunity to elucidate the importance of lateral flow. Sensitivity experiments were performed by varying soil depth, rooting profile, atmospheric driving force, and hydraulic anisotropy ratio to evaluate the hydrologic response to drought.

Poster# 89

NGEE-Tropics: Recent Remote Sensing Campaign in Puerto Rico

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An airborne remote sensing campaign was conducted in March 2017 to link existing field information with new data from the NASA Goddard's Lidar, Hyperspectral, and Thermal (G-LiHT) Airborne Imager. The objectives of the campaign are to (i) characterize carbon stocks in second-growth forests, (ii) investigate leaf chemistry and plant traits, (iii) quantify changes in forest structure in sites with previous lidar coverage, and (iv) facilitate collaborations with ongoing studies in Puerto Rico. We collected remote sensing data across gradients of soil fertility, climate, and forest age. In this poster we present examples of the remote sensing data, flight lines, field plots, and some early look results. This project is a collaboration between DOE, the US Forest Service, and NASA.

Poster# 90

Overview of Research Activities at the K34 Site in Manaus, Brazil: Long-Term Datasets and New Data Collection Initiatives

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Located in the Cuieiras Biological Reserve, about 60 km North of Manaus, Brazil, the K34 site is an intact area in the Amazon tropical forest. The site has been studied for decades, with research activities intensifying after the installation of a 50 m tall tower in 1999. The tower and the surrounding area are well instrumented and data have been collected and used to answer questions ranging from effects of drought, to seasonality of photosynthesis, to carbon assimilation potentials, among many others. These long records of data are invaluable to address questions about long-term effects of climate change, inter-annual variability of vegetation productivity, and validation of long running remote sensing time series, to name a few. Recent additions in research focus and data collection activities are enabling further development of the state-of-the-art in tropical research. In particular, the site is now one of the pilot study sites for the NGEE-Tropics project, and joint research activities are already leading to new insight into effects of a warmer climate, changes in wind regimes, and better understanding on mechanisms regulating emission of volatile organic compounds. This poster will show a summary of the ongoing research efforts at the site, highlighting recent results obtained from long-term datasets and new data collection activities and also opportunities for further investigation.

Terrestrial Ecosystem Science

**Lawrence Berkeley National Laboratory
AmeriFlux Management Project**

Poster# 64

The AmeriFlux Management Project: Overview, Outreach, and Online Activities.

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The AmeriFlux network is a community of sites and scientists measuring ecosystem carbon, water, and energy fluxes across the Americas using eddy covariance techniques. AmeriFlux datasets, and the understanding derived from them, provide crucial linkages between terrestrial ecosystem processes and climate-relevant responses at landscape, regional, and continental scales.

The AmeriFlux Management Project (AMP) was established by DOE in 2012 to support AmeriFlux and the use of its data by a broad community. We work to advance the value of the network for basic research and Earth System Model improvement, innovative measurements, and data synthesis. AMP has teams dedicated to four tasks: Core site support; Technical support and QA/QC; Data support and QA/QC; and Outreach. These efforts are paying off.

The AmeriFlux network is strong and growing. Since 2012, the number of AmeriFlux sites has nearly doubled, to 261, with more sites outside the U.S. and in underrepresented ecosystems. Likewise, the number of site-years of data in the archive increased by 50%. Still, many sites have not yet submitted their data, and we are working with them. AMP is supporting operations for 14 clusters of long-term flux sites, maintaining the continuity and accessibility of these time series. The AmeriFlux Science Steering Committee is operating under a new, more independent charter. In collaboration with ICOS (Europe) and FLUXNET (global) networks, in the past year we completed the release of the FLUXNET2015 dataset for synthesis research. See the Data team poster for more on data processing and products, and the Tech team poster for results from the IRGA intercomparison and tests of sonic anemometers.

In addition to technical and data progress, AMP engages the AmeriFlux community. At the Data-Tech Workshop, held with the 2016 PI meeting in Colorado, attendees worked with the tech and data teams to improve data processing at the site-level and data reporting. AMP incorporated feedback from community members to implement several website improvements. Flux sites can be now searched through maps, keywords, and multiple filters. Site sets can be created to access frequently queried sites with a single click. Each AmeriFlux site's webpage now contains not only general site information but also a newly implemented DOI for each site's data, Data Usage Log, Publications, Imagery, and access to Biological, Ancillary, Disturbance, and Metadata (BADM) information. Two major improvements are an online interface allowing a site's general info BADM to be updated easily and immediately, and publications can be added to the publication database using only the article DOI if desired. This poster will provide highlights of recent outreach and user-experience activities and accomplishments, and solicit input on how we can continue to improve our service to data contributors and data users.

Poster# 65

Updates from the AmeriFlux Tech Team

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The goal of AmeriFlux is to develop a network of long-term CO₂ flux sites for quantifying and understanding the role of the terrestrial biosphere in global climate and environmental change. The AmeriFlux Management Program (AMP) Tech Team at LBNL strengthens the AmeriFlux Network by (1) standardizing operational practices, (2) developing calibration and maintenance routines, and (3) setting clear data quality goals. In this poster we will present results and recent progress in three areas:

- **IRGA inter-comparison experiment:** We simultaneously deployed five gas analyzers commonly used for the Eddy covariance technique from LI-COR, Campbell Scientific, and Picarro, Inc. in an alfalfa field in Davis, CA for a year in order to directly compare the performance of each instrument. Specifically, we compared CO₂ and H₂O mixing ratios, spectral attenuation, and measured fluxes; and analyzed the effect of two spectral corrections commonly applied to fluxes.
- **Gill sonic anemometers:** In late 2015 and early 2016, we uncovered a firmware problem in the Gill WindMaster Pro sonic anemometers used by many researchers for eddy covariance flux measurements. Gill has addressed this issue and has since sent out a notice that the vertical wind speed component (a critical piece of all eddy covariance fluxes) was being erroneously computed and reported. The problem (known as the w-boost bug) resulted in positive (upward) wind speeds being under-reported by 16.6% and negative (downward) wind speeds being under-reported by 28.9%. We are also currently conducting an experiment at US-GLE (Glacier Lakes Ecosystem Experiments Site) to better characterize Gill sonic anemometer transducers shadowing, and define and empirical correction for this shadowing.
- **Unmanned aerial systems (UAS) at AmeriFlux sites:** We will systematically deploy UAS during Tech Team site visits, starting in 2017, and collect visible and pseudo-NDVI imagery using a DJI Inspire-1 drone equipped with (1) a Zenmuse X3 camera with a 20mm focal length for visible imagery, and (2) a Zenmuse X3 camera, modified to filter solely Red + NIR to estimate “pseudo-NDVI” imagery.

Poster# 66

AmeriFlux Data Product and Interface Improvements

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The AmeriFlux Management Project (AMP) Data Team concentration is on providing high-quality, consistent data products from across the flux towers in the Americas. The data team provides a wide array of services to the flux tower teams and data users including: an archive, QA/QC processing, DOIs, and standardization of flux data. In this poster, we will introduce some of the recent advances that are described below.

The AmeriFlux Data Team is developing a new, expanded QA/QC data-processing pipeline and a new standardized half-hourly flux data submission format (called FPin). The new QA/QC pipeline accepts data from flux-tower PIs in FP-in format and produces data in the FP-Standard half-hourly format (these standard formats were developed over the past year, in a collaboration between AmeriFlux and European Flux networks). This standardization is now allowing automation of the data processing and will enable rapid turn-around of processing and feedback to data submitters. In addition, the standard format provides a means for individual sensors to be included in the data submissions and data products. The AMP data team is working with flux-tower teams to convert their data to the FP-in format. We are also working with CDIAC to convert data from inactive AmeriFlux sites to the standard format. On the order of 45 inactive sites have been translated so far and approximately 20 are still in progress. The new QA/QC processing incorporates many of the checks that were developed in the production of the major synthesis data release, FLUXNET2015, and the FP-Standard data output from the new QA/QC processing will be ready for gap-filling, partitioning, and the next generation of FLUXNET processing.

The Biological, Ancillary, Biological, and Metadata (BADM) templates, used to organize and share non-flux data from tower sites, continue to evolve. The new BADM web submission and update interface allows tower teams to easily provide incremental data submissions and corrections of the site general information BADM data. Our next step is to update additional BADM templates like veg cover and soil. In addition, we are working on new submission formats to improve the ease of collecting and submitting BADM data. In concert with the transition to the FP-Standard format, BADM are being used to collect detailed information about sites' instrument installations. An additional upcoming innovation is a file tracking interface that will enable users to track data submission and processing status. We will provide an update regarding the work to develop new partitioning and gap filling. The data team is continually working to improve the flux-tower PI and user experience within AmeriFlux, and thus the usage of flux data in synthesis as well as the breadth, quantity, and quality of the data available from AmeriFlux.

Poster# 67

Constraining Belowground Carbon Turnover Times in Terrestrial Ecosystems: Insights Gained through Radiocarbon Analysis and Interpretation at AmeriFlux Network Sites

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Land-model data comparisons show that models tend to underestimate mean transit time of carbon in terrestrial ecosystems relative to measurement-based estimates largely through an underestimation of soil carbon turnover times. Radiocarbon measurements of multiple quantified pools and fluxes combined with the belowground carbon and radiocarbon modeling tool, SoilR, can provide more robust estimates for transit times than simple, single pool models reliant on assumptions of steady-state and a single time-lag. In addition, this approach can constrain carbon cycles contributing to measured transit times. Well-instrumented sites provide an excellent opportunity to combine existing data, new measurements, and modeling to constrain terrestrial ecosystem turnover times and the mechanisms behind them. Existing soil radiocarbon and carbon stock data from sites in the AmeriFlux Network are being synthesized and reanalyzed using a belowground carbon radiocarbon-modeling tool, SoilR. Current work focuses on five temperate deciduous forests. Of these, four sites were part of the Enriched Background Isotope Study, a ¹⁴C-enriched litter decomposition experiment, which will provide additional data for SoilR model validation. These observed soil profiles are also being compared to model values from CLM and ALM. Additional data, archived samples, and new sampling sites are of interest for future efforts.

Subsurface Biogeochemical Research

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

Poster #150

Watershed Function SFA: Hydrological and Biogeochemical Dynamics from Genomes to Watershed Scales

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Climate change, extreme weather, land-use change, and other perturbations are significantly reshaping interactions with in 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 predictive understanding of watershed hydrological and biogeochemical functioning is challenging, as complex interactions occurring within a heterogeneous watershed can lead to a cascade of effects on downstream water availability and quality. Although these interactions can have significant implications for energy production, agriculture, water quality, and other benefits valued by society, uncertainty associated with predicting watershed function is high.

The Watershed Function SFA aims to substantially reduce this uncertainty through developing a predictive understanding of how mountainous watersheds retain and release downgradient water, nutrients, carbon, and metals. In particular, the project is exploring how early snowmelt, drought, and other disturbances will influence mountainous watershed dynamics at seasonal to decadal timescales. The Watershed Function project is being carried out in a headwater mountainous catchment of the Upper Colorado River Basin: the East River watershed, which is characterized by significant gradients in elevation, vegetation and hydrogeology. A system within system project perspective posits that the integrated watershed response to disturbances can be adequately predicted through consideration of interactions and feedbacks occurring within a limited number of subsystems, each having distinct vegetation-subsurface biogeochemical-hydrological characteristics. New types of observations and experiments are being carried out across satellite and intensive subsystem sites within the watershed, which are elucidating hydrogeological, ecohydrological, and organic-mineral interactions that influence how a range of subsystems respond to perturbations. An early intensive focus is on snowmelt timing in a Lower Montane study site. A key technological goal is the development of scale-adaptive simulation capabilities that can incorporate genomic information where and when it is useful for predicting the overall watershed response to disturbance. Through developing and integrating new microbial ecology, geochemical, hydrological, ecohydrological, computational and geophysical approaches, the project is developing new insights about biogeochemical dynamics from genome to watershed scales.

Poster #151

Hillslope Characterization, Measurements, and Modeling

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Important segments of the hydrologic and elemental cycles reside between the soil surface and impermeable bedrock, where subsurface biogeochemical transformations are depth distributed and coupled to the atmosphere and river via dynamic fluxes of gases, water and solutes. We have begun a set of integrated studies to elucidate these processes through characterization, experiments, and modeling of a lower montane hillslope that drains into the East River, Colorado.

A 200 m long transect was instrumented at four stations where 10 m deep boreholes were drilled to provide samples and measurements within soil, saprolite, and fractured shale. Surface and depth-resolved subsurface measurements are being obtained of aqueous and gas phase compositions, pressures, and temperatures. Hydraulic potential measurements show strong evapotranspiration influence within the upper 2 m, underlain by baseflow through the fractured shale. Pedotransfer functions developed based on measured unsaturated/saturated hydraulic properties combined with meteorological data/drivers (temperature, rainfall, solar radiation, snow and soil water content) from field meteorological stations will be used to estimate infiltration and groundwater recharge. These datasets will be used as inputs for predictive modeling of East River hydrological and biogeochemical conditions.

Spanning broader scales encompassing the hillslope transect and floodplain, electrical resistivity tomography (ERT) and seismic refraction were used to delineate the major lithological units including weathered and fractured bedrock. An automated time-lapse ERT system and point-scale sensors to monitor changes in water content and fluid conductivity were also deployed to provide information on vertical and lateral dynamics in vadose zone and groundwater.

Carbon inventories from the soil surface down through fractured shale bedrock are being quantified through a suite of solid, aqueous, and gas phase analyses. Combining these analyses with field gas flux measurements, laboratory soil/sediment incubation studies, depth-profiled metagenome and metatranscriptome analyses from five sites along the transect, and determination of pore water fluxes will help develop a comprehensive understanding of hydrologic and biogeochemical controls on the hillslope carbon cycle and its exports to the atmosphere and river.

Geochemical and integrated hydrologic modeling activities are being designed along the hillslope transect to better predict partitioning of water, carbon and nutrient fluxes at the site. Preliminary results from modeling show the impact of subsurface heterogeneity on the water energy balance. Next steps in modeling will involve incorporating more field observations and detailed characterization into reactive transport models and resolving rates and fluxes under temporal perturbations (e.g., storm events).

Poster #152

Ecohydrological Controls on Watershed Function: Quantifying Dynamic Surface-Subsurface Interactions

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Significant shifts in vegetation phenology, composition, and functional traits that affect plant production and biogeochemical cycles are thought to be driven by changing hydrologic regimes and water distribution in mountainous ecosystems. However, changing hydrologic regimes also directly impact biogeochemical cycles, which in turn can feed back to vegetation function and further changes in the hydrologic cycle. Our goal is to determine the mechanisms underlying feedbacks between hydrologic disturbance, vegetation phenology/physiology, microbial metabolism and biogeochemical cycling, and contribute to novel watershed scaling constructs. We are taking advantage of both natural (seasonal, elevation, topographic) and induced (warming, earlier snowmelt) variation in temperature, water availability, vegetation, and microbial metabolism/biogeochemistry to identify process coupling. Prior to the current snow season we have performed baseline characterization of vegetation distributions, soil and subsurface physical, chemical, and biological properties and have installed instrumentation to monitor dynamic hydrologic regimes within selected plots across the East River watershed and associated catchments. Remote sensing and machine learning using training data from hillslope transects was employed to classify vegetation and to quantify distributions of functional types (shrubs, forbs, grass). During a warmer than average fall, we observed leaf expansion for many species across all elevations. To determine how litter chemistry impacts decomposition rates and nutrient inputs, litter bags were deployed and initial litter chemistry determined using infrared spectroscopy, elemental analysis, and isotope ratio mass spectrometry. Litter chemistry varied significantly between functional types, particularly nitrogen, phosphorus, and aromatic content. Autonomous *in situ* measurements of seasonal temperature and water availability from the surface through the root zone in these plots demonstrated the insulating effect of snow cover on soil temperature regimes and feedbacks between surface soil temperature and soil water movement under snow. We are currently monitoring under-snow biogeochemical processes through analysis of gas fluxes, lysimeter fluids, and soil cores in order to determine nutrient mobilization and retention by the microbial community prior to and during snowmelt. The fate of these nutrients and their interactions with vegetation phenology will be studied throughout the spring/summer snowmelt.

Poster #153

Geomorphic Controls on Riparian and River Geochemistry in the East River Watershed

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This section of the Watershed SFA focuses on how river morphology, specifically bedform and active and stranded meanders, impacts the redox processes in the associated sediments and therefore the export of carbon, metals, and nutrients into the river. For the bedform driven exchange effort, we employed a river box model to provide the boundary conditions for a subsurface flow and reactive transport model. A Bayesian approach was used for the river box model that allows gross primary productivity, respiration, and diffusion parameters to vary with season. We constrained the model with data including radiation, barometric pressure, water depth, temperature, pH, DIC, and atmospheric CO₂. Downscaled climate predictions of temperature and atmospheric CO₂ were used to force the models and to compare future and current hyporheic zone processing. Initial model results show that hyporheic zone redox conditions are enhanced over the summer growing season, but highly vary depending on the contributions from snowmelt baseflow.

For the meander focus, we combined sediment characterization and water sampling with reactive transport modeling investigations. Specifically, we collected sediment cores from transects across an active and stranded meander and installed piezometers for groundwater sampling. Both transects are characterized by coarse alluvial material (pebbles-cobbles) overlain by finer grained soil/sediment, however the thickness of the finer grained sediment layer varies from approximately 20-100 cm. Several hot spots of Fe-reduction in sediments were identified, which correlate well with measured dissolved Fe(II). TOC concentrations ranged from 0.36-3.29%, generally decreasing with depth. While $\delta^{13}\text{C}$ concentrations showed relatively little variation among samples, $\delta^{15}\text{N}$ varied significantly (-3.3 to 2.5 ‰) suggesting mixing of different sources of N (e.g., Mancos shale versus plants organic matter). Sediment $\delta^{14}\text{C}$ values ranged from -282 to -788 ‰ and were lower in deeper samples. The low $\delta^{14}\text{C}$ values suggest that shale kerogen may be a significant source of organic carbon in the floodplain.

The aggregated functioning of two active meander was explored using PFLOTRAN, and an integrated a biotic and abiotic reaction network. The three-dimensional model was able to predict the hydrological and biogeochemical fluxes in the subsurface. In particular, simulations results, consistent with observations, showed that nitrate, dissolved oxygen, and dissolved organic carbon values decreased, while iron (Fe (II)) values concentrations increased along the meander centerline transect away with distance from the stream. Results also demonstrated that hyporheic flow paths and sinuosity significantly impacted carbon and nitrogen export into the stream system.

Poster #154

Shale Weathering in the East River Watershed

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Much of the East River watershed is underlain by the Mancos shale, which may release biogeochemically significant quantities of organic carbon, nitrogen, metals, salinity and other constituents through abiotic and microbially mediated weathering reactions. The shale weathering team is assessing the extent and timing of nutrient and metal inputs to the river, identifying the dominant water–rock interaction locations above and below the water table, and developing models for weathering reactions. This work contributes to the organo-mineral and nitrogen cycle components of the SFA research plan.

Work initiated in the 2016 field season performed essential shale characterization, identified candidate water chemistry and isotopic signatures of shale weathering, and installed sampling infrastructure. A 4-inch OD x 8.5-m core from the hillside transect will provide a detailed sedimentary sequence and estimates of fracture density and fracture surface weathering extent with depth. We performed elemental, mineral, and imaging analyses as well as carbon and nitrogen isotope measurements of shale samples from outcrops throughout the watershed and 1” cores drilled from bedrock along the East River. The shale hosts abundant pyrite in forms ranging from dispersed framboidal aggregates, pyritized burrows and millimeter-thick seams. Associated metal sulfides include discrete nanoscale particles of CdS (probably greenockite). Shale water samples showed a high sulfate concentration and $\delta^{34}\text{S}$ of -23‰ indicating oxidation of sedimentary pyrite, providing a tracer for shale-sourced sulfate in the watershed (streams range in $\delta^{34}\text{S}$ from -15 to +5). We installed vertical and horizontal water sampling ports into shale bedrock at several locations to enable monitoring of seasonal variations in water content and chemistry, isotopes including H₂O, Sr, and U, and microbial community composition.

Ongoing and planned work will study shale weathering processes through complementary efforts. Laboratory column studies will assess the effect of shale metamorphism on weathering and carbon release. Batch incubations will assess the potential for carbon and metal release through microbial reactions. Metagenomic analysis of fluids from pyrite-rich locations will establish the communities hypothesized to initiate the weathering process. High-resolution imaging will determine if weathering pathways follow the same sequence in soil- versus ground water-dominated zones. Detailed studies of nitrogen content, speciation and isotopic composition in rock and fluids will evaluate the potential for *in situ* nitrification.

Poster #155

Genome-Resolved Metagenomic and Geochemical Analysis of East River Riparian Zone Soils Supports the 'Systems Within Systems' Approach for Watershed Analysis

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Microorganisms largely control carbon turnover and mediate other important biogeochemical processes in soils. Information regarding microbial impacts at larger spatial scales is required to understand ecosystem processes. Our approach to scaling genome-resolved metagenomics to study the riparian zone was to target discrete reaches of the East River as a potentially representative repeating motif. We are testing this hypothesis using extensive sampling and DNA sequencing based analyses. 94 soil samples were collected over the 10-25 cm depth interval from floodplains associated with three meandering reaches: upstream (MG), midstream (ML), and downstream (MZ). Genomic DNA was extracted and then sequenced at the Joint Genome Institute on a HiSeq Illumina instrument (~ 5 Gbp per sample).

DNA sequence information from individual samples was processed and assembled using standard methods. Based on profiling of community composition using scaffolds encoding *rpS3*, we identified 813 distinct strains, many of which were found at multiple sites within a meander and also occurred in two or all three meanders. Shortly after assembly we have already recovered 164 draft or higher quality genomes representing 88 distinct microorganisms. Most of the relatively abundant organisms in the three systems are represented by draft genomes, the main exception being some members of a group of highly abundant and closely related strains of Betaproteobacteria. For many organisms, the same genome was recovered from multiple samples. For example, for one novel Betaproteobacteria we reconstructed 11 near complete genomes and a genotype of Gammaproteobacteria is represented by 11 genomes. Other groups of abundant, novel, and genomically defined Bacteria include Acidobacteria, Ignavibacteria, Nitrospirae, Gemmatimonadetes, Deltaproteobacteria, Verrucomicrobia, and Planctomycetes. Thaumarchaeota (Nitrosopumilales) were the most abundant Archaea observed in these samples. Additionally, we recovered genomes for a variety of very little understood organisms known only from prior genomic studies, mostly at the Rifle SFA research site. These include Rokubacteria, WS3X, CHLX, Zixibacteria, OD1 (various Parubacteria), and DPANN (Pacearchaeota). Widely distributed functions in addition to carbon turnover include sulfur oxidation, iron oxidation, ammonia oxidation, nitrate reduction, and nitrogen fixation. Despite heterogeneity in species distribution, strong overlaps in organism membership and similar functions are well represented across the three localities; however, the function of some organisms may vary across sites. Overall, we conclude that genome-resolved metagenomics, analyzed in the context of physical and chemical information, can be scaled to understand the distribution of ecosystem processes. Insights regarding community composition from a single floodplain may be generalizable, at least under some conditions.

Poster #156

Digital Watershed: Advanced Watershed Characterization across Scales

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Predictive understanding of watershed function and dynamics is often hindered by the heterogeneous and multiscale fabric of watersheds. In particular, biogeochemical cycling involves complex hydrological-biogeochemical interactions occurring from bedrock-to-canopy, including plants, microorganisms, organic matter, minerals, dissolved constituents, and migrating fluids. Understanding and quantifying such interactions across heterogeneous watersheds is critical for estimating and predicting integrated ecosystem responses – such as carbon and nutrient export and impacts to water quality – under climate changes and other perturbations.

Under the Watershed Function SFA, we develop novel watershed-characterization methodologies 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 and remote sensing data, we catalyze the development of the fundamental scientific linkages among interacting processes in the watershed. Particular focus is to quantify and distribute subsurface and biogeochemical properties by exploiting their co-variability with geomorphology and vegetation (i.e., plant functional types and their dynamics) that can be measured by remote sensing. First, we couple surface geophysics (seismic and electrical) and multiple remote sensing (i.e., airborne LiDAR, UAV) to quantify the co-variability between geomorphology and subsurface structure, and then to estimate the bedrock depth and other subsurface properties across the watershed. Second, we develop an advanced data fusion and machine learning-based approach to estimate the plant functional types and traits over the watershed in high-resolution by integrating multispectral images and airborne LiDAR. The detailed distributions of plant characteristics are then used to scale biogeochemical properties across the watershed. By characterizing heterogeneous properties over the watershed, we aim to develop the new ‘Digital Watershed’ concept for model parameterization and validation.

Poster #157

Observing and Modeling Snow Processes Across Spatial and Temporal Scales in a Rocky Mountain Headwater Catchment

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In high elevation catchments of the western United States, snowmelt supports downstream populations, provides ecosystem services, and drives critical zone water, nutrient, and metal fluxes and transformations. Changing climatic conditions are challenging our current conceptualization of processes that govern snow accumulation and melt over seasonal and decadal timeframes, with studies performed as part of Berkeley Lab's Watershed Function Scientific Focus Area addressing these challenges through observational and modeling studies conducted in the East River watershed in Central Colorado. Recent work has found that snow formulations in physically-based land surface models perform poorly in the Rocky Mountains; a finding which may be attributed to complex terrain and vegetation heterogeneity that is not captured at larger scales. Here, we combine modeling with airborne and ground observations of snow at high resolution to characterize its role in controlling critical zone processes. We validate the land surface model in ParFlow-CLM using locations with co-located meteorological and snow observations to understand the parameters driving precipitation partitioning, sublimation, and snowmelt. Hourly simulations are run for nearly a decade to evaluate model performance with variable precipitation conditions at high temporal resolution and to explore the effects of altered precipitation patterns with climate change. To fully understand snowmelt across spatial scales in complex terrain, the land surface model is applied to the ca. 300-km² East River watershed over elevations ranging from 2700-3900m and life zones from montane to alpine. Model outputs are interpreted using LiDAR overflights of the ground surface (0.5m lateral resolution) and maximum snow depth (3m lateral resolution) to characterize high resolution topography and snow loading. Remote observations of snow are complemented by extensive ground sampling to improve estimations of snow density and quantify uncertainty. The combination of point-scale observations and model evaluation with high resolution modeling and airborne data collection provides new insight into snow processes from the plot to watershed scale. This combined approach uses modeling to bridge the gap between the spatial and temporal limitations of observations. In turn, observations contribute confidence that physical processes important to snow accumulation and melt are captured in the model, which offers a test bed for understanding snow-driven processes across the critical zone, from bedrock through the canopy.

Poster #158

Nested EMMA to Identify Stream Sources in a Colorado River Headwater Catchment

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Stream concentration-discharge relationships represent an integrated hydrologic response of the individual catchment with a direct link to contributing sources, associated flow paths and groundwater residence times. We employ the empirical approach of end-member mixing analysis (EMMA) using a suite of natural chemical and isotopic observations within the East River, CO; a snow-dominated, headwater catchment of the Colorado River and recently designated as the Lawrence Berkeley National Laboratory Watershed Function Science Focus Area study site. EMMA relies on eigenvector and residual analysis and is used to estimate mixing model dimensionality and identify contributing end-members of the furthest downstream (84.7 km²) and most heavily characterized stream gauge in the study site. Model development using this gauge helps minimize uncertainties related to sampling frequency, temporal variability, and possible data gaps. Results are then applied to 10 nested sub-catchments (ranging from 0.38 km² to 69.9 km²). The mixing space will scale if the seasonal ratios among solutes are maintained. In contrast, lack of a common mixing subspace will occur if water originates with a different chemical signature, contacts and exchanges solutes with different mineral assemblages, or experiences dissimilar hydrologic partitioning. We discuss similarities and differences in the predictive power of EMMA among sub-catchments in terms of first-order geospatial characteristics and with reference to processes that potentially violate underlying assumptions of linearity in mixing and conservative behavior of tracers. Nested EMMA is an initial step to elucidate source contributions to streamflow and address scalability and applicability of mixing processes in a complex, highly heterogeneous, snow dominated catchment. Work will aid hydrologic conceptualization of the East River, guide future observation, and inform numerical model development over a range of scales and across key system subcomponents, such as hillslopes, floodplains, and deep groundwater.

Poster #159

Spatial and Temporal Dynamics of Carbon and Nitrogen within a Mountainous Watershed

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Mountainous watersheds are characterized by substantial heterogeneity in geomorphology, soil texture, and vegetation that determine hydrological flow paths and residence times through distinct catchment subsystems. Despite advances in understanding of the spatial and temporal drivers of biogeochemical cycling within snowmelt-dominated ecosystems, knowledge gaps remain. Here we describe ongoing work examining the input, transformation, and export of carbon and nitrogen within the East River (CO) catchment, with a focus on data collected from one catchment subsystem, a lower montane meadow intensive study site, since the project started in Fall 2016. With respect to carbon, initial work seeks to characterize the depth- and time-resolved distribution, inventories, and fluxes of soil carbon from surface soils through fractured and consolidated bedrock to a depth of 10 m. We will show data for organic and inorganic carbon content and corresponding isotopic signatures (¹³C and ¹⁴C) in soil, soil extracts, and pore water samples collected along a hillslope-to-riparian floodplain transect across a lower montane meadow. Respiration rates and metagenome/metatranscriptome profiles will also be included. Additional ongoing work at the lower montane site focuses on seasonal trends in established vegetation plots and aims to elucidate, in particular, N biogeochemical cycling during snowmelt in this subsystem and the effects of early snowmelt. Presented baseline data will encompass: soil gas fluxes (CO₂, CH₄, and N₂O, including under-snow measurements), soil microbial biomass (C and N, and their corresponding isotopic signatures), associated microbial community composition, and soil NH₄⁺, NO₃⁻, and P concentrations (the soil data covers multiple depths). This and other work builds toward the broader SFA goal of the “Nitrogen Milestone”. Nitrogen is a major limiting nutrient within mountainous regions and the current work focuses on a high-resolution, cross-watershed characterization of the nitrogen cycle during different hydrological regimes (baseflow, snowmelt, drought, and monsoonal precipitation). High frequency NO₃⁻ measurements have been made over the past two years, both within the East River and in several tributaries, and reveal NO₃⁻ fluxes that span nine orders of magnitude across the catchment; work with the stable isotopes (δ¹⁵N and δ¹⁸O) of NO₃⁻ continues to link this data with specific biogeochemical drivers. Overall, such baseline data on input, transformation, and export of nitrogen and carbon from catchment subsystems will be used to inform modeling efforts and contribute to scale-adaptive approaches to represent the feedback between hydrological perturbation and biogeochemical processes to improve predictions of nitrogen export from the catchment.

Poster #160

Scale-Adaptive Watershed Simulation of Watershed Function

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The Watershed Reactor Component of the Watershed Function SFA is pursuing a set of modeling activities to quantify key controls on watershed system behavior driven by coupled hydrologic, vegetation and biogeochemical parameters. The modeling tasks are motivated by the need to quantify water and nutrient fluxes into, cycling within, and export from interconnected hydrologic units without undue sacrifice of resolution and process fidelity.

A key task within this component focuses on bringing vegetation models into hydrological codes (ATS, ParFlow) to account for water, carbon, nitrogen cycling by means of a generic interface. Other modeling activities focus on floodplain meanders near the East River Pump House, where data indicate nitrification and Fe(III) reduction to Fe(II) across <1m spatial scales. Bedform data show complete oxygen consumption over a 10cm vertical scale in the riverbed. Models developed with these data are currently being tested to assess how early snowmelt conditions will influence key redox controls on carbon and nutrient budgets. A two-dimensional transect is used to demonstrate how hyporheic flow paths within an intra-meander region impact carbon and nitrogen export into the stream system. Efforts are also underway to upscale the local carbon cycling displayed with individual stream meanders to the larger East River system, in part by making use of the high performance computing platform provided by PFLOTRAN and ATS.

Another activity in collaboration with the Hydrology Component of the Watershed Function SFA involves high resolution hill slope modeling of an instrumented transect. The hill slope modeling, which will eventually consider the chemical weathering of the shale over geologic time, will be paired with the floodplain modeling to develop mesoscale models for water and nutrients. Comparisons of fluid residence times of two mesoscale models, a high-elevation upper montane and a low-elevation floodplain site, will be used to explain differences in carbon exports measured in the field. This mesoscale modeling effort will serve as the basis for a more comprehensive scale-adaptive approach that will consider parallel-in-time fine and coarse scale watershed simulations.

A 10m resolution integrated hydrologic model of the East River has been developed to test hypotheses and guide observations. Watershed scale model resolution is varied over 2 orders of magnitude across all 255km², from a near-observational scale (10m) to a regional modeling scale (1km), providing an opportunity to bracket uncertainty in projected environmental changes and to determine the scale at which functional hydrologic relationships break down.

Poster #161

LBNL Watershed SFA Data Management and Assimilation

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The objective of the Data Management and Assimilation (DMA) component of LBNL's Watershed Function SFA is to enable science by addressing the priority data science needs of the SFA team. The heterogeneous data sets collected at the East River site include over 80 different data types and includes hydrological, geochemical, geophysical, microbiological and remote sensing data. This data is being collected from a number of different sources. This includes data collection directly funded by the SFA (e.g. data from instrumented sensors, geochemical sampling efforts and remote sensing campaigns), data collected by a broad range of collaborators, and data from 3rd party sources (e.g. USGS streamflow and NRCS SNOTEL data). This data needs to be used as inputs for analytical and numerical modeling of the meteorological and hydrological water balance, including infiltration and groundwater recharge, as well as an evaluation of long-term trend of climatic conditions and nutrients balance.

The DMA team has developed a number of tools for automated data QA/QC, data ingestion, data exploration, data preservation, and data distribution. Automated data QA/QC is performed using statistical to identify and flag issues in the datasets. Data integration is achieved via a brokering service that dynamically integrates data from distributed databases via web services, based on user queries. The integrated results are presented to users in a web portal that enables intuitive search, interactive visualization and download of integrated datasets. Data preservation and distribution are being enabled by a web portal that allows authorized users to upload and download data files as packages. The DMA team is also building an interactive map of data collection sites run by the SFA and its collaborators, to inform the broader community about SFA field activities (the map is featured in the Watershed SFA Community Observatory page of the SFA website). Sites can be filtered by their key measurements and other metadata, leading to detailed site landing pages.

The data are used for building crosscutting data products needed for the hypothesis testing and numerical modeling of hydrological and biogeochemical conditions of the East River watershed by the SFA project teams. For example, we are analyzing a set of meteorological model drivers (temperature, rainfall, solar radiation, snow depth, snow water content, etc.) from a network of meteorological stations, and the river discharge from field observations along the East River.

Subsurface Biogeochemical Research

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

Poster #173

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 the processes that govern influences of hydrologic exchange flows on water quality, nutrient dynamics, and ecosystem health in dynamic river corridor systems. Exchange of water between rivers and the surrounding subsurface environments (hydrologic exchange flows or HEFs) are a vital aspect of watershed function. HEFs lead to enhanced biogeochemical activity (accounting for up to 96% of respiration within river ecosystems) 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, particularly in the context of large managed rivers with highly variable discharge, and are poorly represented in system-scale quantitative models. Using the 75 km Hanford Reach of the Columbia River as our research domain, we have developed fundamental understanding in several areas including i) effects of groundwater-surface water mixing on ecological assembly processes, biogeochemical rates, and balance among metabolic pathways, ii) river water pathways and impacts on contaminant plume mobility, iii) physical controls on HEFs at kilometer scales, iv) impacts of microbial regulation processes on biogeochemical rates in response to changing environmental conditions, and v) the nature, speciation, and energetics of organic carbon driving biogeochemical processes. We established a facies-based multiscale simulation approach to incorporate new understanding into predictive models. Proposed research will build on this foundation to develop a fundamental and comprehensive scientific understanding of the influences of HEFs (in particular as driven by river discharge variations) on river corridor biogeochemical and ecological functions and to integrate this new-found scientific understanding into a first-of-kind hydrobiogeochemical model of the river corridor, linked as a critical component of watershed systems models. Accordingly, we will pursue the resolution of fundamental scientific hypotheses designed to advance understanding of coupled hydrobiogeochemical processes. At the same time, we will develop a hierarchical multiscale modeling framework that will integrate scientific understanding into a predictive watershed modeling capability with wide applicability. New predictive understanding of HEFs and biogeochemistry in the river corridor will play a key role in reduction of uncertainties associated with major Earth system biogeochemical fluxes, improving predictions of environmental and human impacts on water quality and riverine ecosystems, and supporting environmentally responsible management of linked energy-water systems.

Poster #174

Quantifying Reach-Scale Hydrological Exchange Flows and Their Influences on Biogeochemistry, Contaminant Mobility, and Land-Surface Fluxes

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This element of the PNNL SBR SFA seeks to quantify the cumulative effects of hydrological exchange flows (HEFs) on reach-scale phenomena (i.e., water quality, nutrient dynamics, and ecosystem health) in dynamic river corridor systems, based on rigorous upscaling of mechanistic process understanding developed at hydromorphic units. HEFs in rivers play vital roles in watershed ecological and biogeochemical functions due to their strong capacity to attenuate contaminants and process significant quantities of carbon and nutrients. Recent PNNL SBR SFA studies, using a combination of numerical simulations and field observations, have revealed complex spatial and temporal dynamics in km-scale HEFs and their significant impacts on contaminant plume mobility, hyporheic thermal regimes, and land surface energy fluxes at a few km-scale sites along the Hanford Reach. The coupling between massively parallel flow and reactive transport code PFLOTRAN and the Community Land Model (CLM), PFLOTRAN_CLM, provides a key capability for studying the interactions between river water, groundwater, and land surface processes.

Expanding on these previous research, we propose to conduct field and numerical experiments to evaluate the influence of HEFs on riparian-zone biogeochemistry, land surface fluxes, and contaminant mobility at the scale of the entire Hanford Reach (10s of km). This activity will develop reach-scale flow and reactive transport (PFLOTRAN) model using unstructured variable-resolution grids, incorporating reduced-order models of HEFs and nitrogen cycling developed from high-resolution mechanistic models at hydromorphic units. The nitrogen cycling will be informed by spatially distributed carbon stocks mapped from remotely sensed measurements and the ultra-high resolution carbon characterization. The resulting model system will be applied to quantify carbon/nitrogen dynamics and contaminant transport and transformation at the Hanford Reach scale, as a representative example of influences of HEFs on system-scale biogeochemistry. The flow and reactive transport model will be calibrated against both site-wide contaminant monitoring data and new spatially distributed HEF measurements. The coupled PFLOTRAN_CLM model, informed by eddy-covariance measurements of latent heat and carbon fluxes from three flux towers distributed across the Hanford Reach, will be used to assess the impacts of HEF on riparian vegetation and land surface fluxes. This activity will be heavily informed by a combination of high-resolution mechanistic models and process studies across the SFA project. The upscaling of mechanistic processes from the hydromorphic scale to reach scale will fill in a critical need in bridging the gaps between hydromorphic-scale process understanding and robust predictions of the watershed hydrobiogeochemical function.

Poster #175

Cumulative Effects of River Corridor Hydrobiogeochemical Processes on Watershed Functioning

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This element aims to assess cumulative effects of river corridor hydrobiogeochemistry on nutrient (N, C) balance at reach and watershed scales, and quantify the relative contributions of large mainstem river corridors to watershed scale nutrient budgets. We will develop a first-of-kind river corridor model capable of representing hydrologic exchange fluxes (HEFs) and associated biogeochemical processes guided by high-resolution mechanistic model simulations. This new river corridor model will be coupled with other existing watershed model components to create a prototype watershed-scale modeling framework that directly accounts for river corridor hydrobiogeochemistry in predictions of watershed-scale nutrient processing, water quality, and ecosystem health. In previous research, we have established a coupled modeling framework featuring the coupling of the subsurface flow and reactive transport code PFLOTRAN and the Community Land Model (CLM) for studying interactions among groundwater–surface water–land surface processes. We also collected hydrogeological, riverine, land surface, and hydro-climatic datasets along the Hanford Reach and beyond, and assessed the role of water management activities, such as reservoir operation, on regulating river discharge along the Hanford Reach. Built upon these efforts, we will couple three models representative of river corridor processes: subsurface flow and reactive transport (PFLOTRAN), land surface processes (CLM), and river flow and transport (i.e., the routing model in the Soil and Water Assessment Tool [SWAT] or SWATR hereafter) enhanced with hydromorphology-based models of hydrologic exchange and reaction potential (i.e., the physically-based Networks with EXchange and Subsurface Storage or NEXSS). A new version of NEXSS will be created to incorporate a detailed hydromorphic classification scheme and estimates of HEFs and residence time distributions based on mechanistic model results. SWATR will be modified to incorporate a multi-rate transient storage model and reactions. In parallel to model development, cumulative effects of hydrologic exchange flows and river corridor biogeochemistry on watershed-scale nutrient processing will be evaluated by conducting numerical experiments in the Upper Columbia-Priest Rapids watershed using SWAT with and without river corridor HEFs. The modeling of HEFs and associated biogeochemical processes will be enabled by the coupled SWATR-NEXSS model. This will lay the foundation for applications of the prototype coupled watershed modeling framework. The proposed model development activities will benefit greatly from the fundamental knowledge regarding river corridor HEFs and biogeochemistry derived from mechanistic models and observations from other research elements. Meanwhile, our research team will collaborate with the DOE IM³ SFA to leverage their developments in watershed-scale modeling with reservoir impoundments.

Poster #176

Quantifying Stream-Aquifer-Land Interactions Along the Columbia River Corridor Using Integrated Modeling and Observations

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In this element, stream-aquifer interactions in terms of variations in mass exchange rates and groundwater elevations induced by pressure gradient and mass exchange along the Hanford reach of the Columbia River Corridor, as well as their relations to the partitioning of the surface energy budget were quantified, by developing and applying an integrated surface and subsurface model, and analyzing observations from two eddy-covariance tower sites. The integrated model features the coupling of the Community Land Model version 4.5 (CLM4.5) and a massively-parallel multi-physics reactive transport model (PFLOTRAN). The coupled model, named PFLOTRAN_CLM v1.0, was applied to a 400 m×400 m study domain along the Columbia River shoreline and validated against observations from groundwater monitoring wells. PFLOTRAN_CLM v1.0 simulations were performed at three spatial resolutions over a five-year period to evaluate the impact of hydro-climatic conditions and spatial resolution on simulated variables. Our numerical experiments suggested that the land-surface energy partitioning was strongly modulated by groundwater-river water exchanges in the periodically inundated fraction of the riparian zone, and enhancing moisture availability in the vadose zone via capillary rise in response to the river stage change. Furthermore, spatial resolution was found to impact significantly the accuracy of estimated the mass exchange rates at the boundaries of the aquifer, and it becomes critical when surface and subsurface become more tightly coupled with groundwater table within six to seven meters below the surface. The findings from model simulations were confirmed by observations from two eddy covariance flux towers. Preliminary analyses of tower measurements suggested that land surface energy fluxes and net ecosystem exchange could vary significantly as a function of accessibility to groundwater and its connectivity to river water. The coupled model developed in this study can be used for improving mechanistic understanding of ecosystem functioning, biogeochemical cycling, and land-atmosphere interactions along river corridors under historical and future hydro-climatic changes, including river reaches downstream to hydropower dams characterized by highly variable river stage variations. The dataset presented in this study can also serve as a good benchmarking case for testing other integrated models.

Poster #177

Functional Enzyme-Based Approach for Modeling Aerobic Respiration Processes in Hyporheic Zone Sediments Subject to Variable Inundation History

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This element of the PNNL SFA seeks to understand the control exerted on biogeochemical reactions by hydrologic exchange flows and translate that understanding into predictive genome-informed biogeochemical process models. Seasonal and inter-annual changes in large-scale water supply, combined with the modulating influence of highly variable releases from hydropower facilities, can give rise to large changes in river surface elevation (stage) across a spectrum of time scales. Therefore, riverbed sediments in the parafluvial zone are continually subjected to cycles of inundation and drying. SFA research has recently revealed that organic carbon speciation and transformation rates depend on time lags in aerobic respiration associated with inundation history. We have also developed a new enzyme-based biogeochemical modeling approach that accounts for microbial regulation, and successfully applied that approach to simulate denitrification processes. Proposed research will develop new and modified reaction models that will account for thermodynamic principles as well as fundamental biological mechanisms responsible for metabolic response lags. These reaction networks will be expanded from our current denitrification model to represent processes governing carbon speciation and transformations, and will involve redox pathways of nitrogen and other secondary metabolites to complete reaction paths. Based on the reasoning that biogeochemical dynamics are related to compositional status of a microbial community, we will split the community population into multiple (initially two) microbial groups characterized by different dynamic time scales: 1) oligotrophs that preferably grow at low concentration of nutrients and show long time lags and 2) copiotrophs that preferably grow at high concentration of nutrients and show brief time lags. Processes governing historical contingencies will be represented in terms of microbial response lag as a function of relative abundance of these two groups, which will vary depending on the inundation history. Reaction model development will be informed by new understanding from FTICR-MS carbon characterization, microbial genome annotation and analysis, and field-based process studies, and the resulting models will be incorporated into high-resolution reactive transport simulations of biogeochemical processes in canonical hydromorphic structures. Those simulations will enable translation of new fundamental process knowledge into predictive understanding of system behavior at larger scales.

Poster #178

Influences of Hydromorphic and Hydrogeologic Structure and Variable River Discharge on Hydrologic Exchange Flows and Biogeochemical Transformations in the River Corridor

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This element of the PNNL SFA seeks to understand the influences of hydromorphology and hydrogeology as they interact with variable river flows to control hydrologic exchange flows and associated biogeochemical processes. Hydromorphic structure of the river channel, and hydrogeologic heterogeneity of the underlying riverbed and aquifer sediments, interact with variable river discharge to control the exchange of river water and groundwater (hydrologic exchange flows or HEFs) in ways that are not yet well understood. HEFs stimulate biogeochemical activity which influences water quality (temperature and contaminant removal) and nutrient balances. Recent SFA research has developed and validated an approach that quantifies large-scale HEFs using local temperature measurements to inform and constrain simulations of HEFs using 3D computational fluid dynamics (CFD) modeling, with river flow and the inland water table as boundary conditions. To assign physical properties for the CFD models, we used high-resolution bathymetry from Light Detection and Ranging (LiDAR) surveys and riverbed grain size from underwater camera image analyses and sediment samples. These studies revealed that HEF direction and magnitude are controlled by the river discharge and are highly sensitive to the thickness and properties of the biologically active alluvial layer that forms the first few meters of the riverbed. Proposed research will expand these results to a number of characteristic hydromorphic settings, using our facies-based characterization approach and linked to field observations of HEF, geophysical surveys, and reactive tracer tests. New research will elucidate the impacts of poorly-understood and critical factors (temporally variable discharge, subsurface heterogeneity, and regional groundwater flow) on HEF and associated biogeochemistry through a series of numerical experiments. These will be based on high-resolution CFD simulations linking transient river flow to HEF and predicting subsurface residence time distributions. New reaction models that account for microbial regulation processes and community dynamics will be incorporated into reactive transport simulations to account for impacts of carbon sources and speciation as well as inundation history. Results of these simulations will guide formulation of reach-scale reduced-order models and parameterizations that will build new predictive understanding and simulation capability applicable at river network and watershed scales.

Poster #179

Low Flow Conditions Maximize the Impacts of High-frequency River Dynamics on Hyporheic Biogeochemical and Thermal Exchange

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This element of the PNNL SBR SFA aims to understand how the high-frequency flow variations control the temperature dynamics and biogeochemical fluxes within the hyporheic zone. Hydroelectric dams tend to increase the frequency of river stage fluctuation due to the relatively short temporal cycles of power production, while they also moderate extreme seasonal fluctuations with their ability to store and release water. However, little is known regarding the secondary impact of dam-induced flow variations on downstream hyporheic zone activity. In this research, hyporheic zone biogeochemistry and temperature were studied under variable flow regimes ranging from natural river flow (i.e. no dams) to high-frequency reservoir release common to power production. Natural river flow was synthetically generated by removing high-frequency fluctuations (e.g. subdaily). Hydrogeologic properties for this study were based on the Hanford 300 Area conceptual model with a high permeability Hanford Unit, underlain by a low permeability Ringold Unit and covered by a fine-grained, low permeability sediment at the riverbed. A vertical two-dimensional cross section was developed with a high resolution (10cm x 5cm) grid near the river. Hyporheic zone hydrologic and thermal flows were modeled through PFLOTRAN's thermo-hydrologic flow mode. Carbon consumption (i.e. aerobic respiration, denitrification, and biomass production) was simulated through a cybernetic reaction network with temperature-dependent rate constants developed within the PFLOTRAN reaction sandbox.

The multi-year (2010-2015) simulated exchange of energy and carbon mass within the hyporheic zone revealed that high-frequency stage fluctuations had their strongest thermal and biogeochemical impacts when the mean river stage was low. Seasonal decreases in river stage therefore coincided with the greatest impacts; the largest impacts were normally in the early winter when high frequency fluctuations cooled the hyporheic zone. An abnormally low snowpack in 2015, however, caused low river stage during summer months. The resulting high-frequency stage fluctuations at low river stage caused the hyporheic zone to warm. The spatial pattern of biogeochemical hot spots was found to highly depend on the heterogeneity in subsurface hydraulic properties instead of flow variations. This study provides a scientific basis for assessing the potential ecological consequences of high-frequency flow variations in a regulated river. The understanding developed from this study has motivated new research to connect hydrological exchange flows and their associated thermal and biogeochemical processes to mean river stage, frequency of stage fluctuations, and hydrogeology.

Poster #180

Processes Governing the Biogeochemical Consequences of Inundation History and the Character of Dissolved Organic Carbon

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*This element of the PNNL SFA will contribute to a predictive understanding of river corridor hydrobiogeochemical function by revealing processes that govern the biogeochemical consequences of inundation history and the character (e.g., thermodynamic properties) of organic carbon (OC). Hydrologic alterations are ubiquitous across watersheds, and these changes influence inundation dynamics within the parafluvial hyporheic zone. These alterations further impact the quantity and character of OC delivered to the hyporheic zone. Our previous research showed that the history of inundation and OC character strongly influence biogeochemical function within the river corridor. We found that time since last inundation strongly influenced the response of hyporheic zone microbial communities and biogeochemical rates to re-inundation. We also found that inputs of thermodynamically favorable OC protect less favorable, mineral-bound OC from microbial oxidation. In contrast, favorable OC derived from groundwater may stimulate the oxidation of less favorable river-derived dissolved OC. There are, however, significant knowledge gaps associated with processes governing the biogeochemical influences of hydrologic history and OC character. Furthermore, such processes are not represented in reactive transport models. This severely limits our ability to develop process-based models of river corridor hydrobiogeochemical function, especially under conditions of altered hydrologic regimes. We will therefore build from our previous work to evaluate hypotheses associated with the biogeochemical influences of inundation history and OC character across a range of variable river stage conditions and physical settings. We will rely on manipulative field experiments within three major hydromorphic settings distributed across the Hanford Reach of the Columbia River. Experimental design will be informed by reactive transport models that include new reaction network formulations representing hypothesized influences of history and OC character. The experiments will leverage well-characterized spatial patterns in inundation history to examine associated influences, and use *in situ* reactive tracer injections to study controls over and influences of OC character. Following manipulations of hydrologic history, biogeochemical and microbial responses will be assayed using advanced analytical and molecular tools. Influences of OC character will be evaluated by injecting OC solutions with known concentration and thermodynamic properties into the subsurface and measuring biogeochemical responses with co-injected reactive tracers. The work will involve significant molecular characterization, leveraging ESML and JGI. Resulting knowledge will be translated into predictive reactive transport models using an iterative model-experiment approach. Resulting process-based models are a critical component of the predictive watershed-scale modeling framework that will be delivered by the PNNL SFA.*

Poster #181

Interactions Between River Stage Dynamics and Physical Setting on Hydrologic Exchange Flows and Primary Producer Biomass within the River Corridor

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This element of the PNNL SFA will contribute to a predictive understanding of river corridor hydrobiogeochemical function by revealing interactive influences of river stage dynamics, hydromorphic setting, and hydrogeologic heterogeneity on hydrologic exchange flows (HEFs) and associated biogeochemical function. In the U.S. 90% of water discharge is hydrologically altered, whereby river stage dynamics are continually perturbed. There is a pressing need to understand how hydrologic alterations impact HEFs due to zones of hydrologic exchange contributing up to 96% of metabolism in riverine ecosystem. This project will, therefore, fill a fundamental knowledge gap that impedes progress towards process-based watershed management. Previous simulations indicated that the influence of variable discharge on HEFs will result from interactions between mean river stage and river stage dynamics. We hypothesize that hydromorphic setting will combine with these interactions to govern HEFs. In addition to evaluating this hypothesis we will characterize features of the river corridor system needed to setup hydrobiogeochemical models. These features include the three-dimensional structure of subsurface hydrogeology and reach-scale spatial distributions of primary producer biomass and associated carbon stocks. For hypothesis testing and feature characterization we will leverage a spatiotemporal mosaic of river stage variability, hydromorphology, and hydrogeology throughout the Hanford Reach of the Columbia River. Field sites will be distributed across ~100 km to study a continuum of variable river stage fluctuations and physical characteristics. Discrete field sites will focus on characterization of HEFs using *in situ* temperature and pressure sensors. In select sites we will also characterize hydrogeologic structure and *in situ* biogeochemical rates across river stage conditions using a combination of conservative salt tracer and reactive tracer injections into the subsurface. Salt tracer will act as a contrasting agent for time-lapse electrical resistivity tomography (ERT). To infer hydrogeologic structure, ERT surveys will be analyzed using the hydrogeophysical inversion code PFLOTRAN-E4D. Time series of reactive tracer concentrations will provide estimates of biogeochemical rates. Those estimates will be linked to hydrogeology, proximity to riparian vegetation, and river stage conditions. In addition, we will use remote sensing and UAV-based data collection via the ARM user facility to estimate spatial variation in aquatic and terrestrial primary producer biomass. Resulting knowledge and data products are integral to the PNNL SBR SFA and will be used in an iterative model-experiment approach to facilitate the calibration/evaluation of mechanistic models at the scale of hydromorphic units and evaluation of reduced-order models at reach to watershed scales.

Poster #182

Organic Carbon Thermodynamics Elucidate Spatiotemporal Mechanisms Governing Hyporheic Zone Biogeochemical Cycling

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This element of the PNNL SFA has contributed to a predictive understanding of river corridor hydrobiogeochemical function by revealing processes governing the oxidation of organic carbon (OC) in the hyporheic zone. Groundwater-surface water mixing zones (i.e., hyporheic zones) exhibit enhanced biogeochemical cycling, and strongly influence river corridor function. Processes governing biogeochemical cycling in these zones remain a crucial uncertainty in watershed-scale process models. To reveal governing processes we combined ultra-high resolution OC characterization, geophysical monitoring, microbial ecology, and biogeochemical assays to determine novel processes associated with the concept of ‘priming’ and how those processes are influenced by (i) riparian vegetation and (ii) hydrologic mixing in the Columbia River hyporheic zone. Here, priming occurs when microbial oxidation of thermodynamically unfavorable OC is fueled by the addition of more bioavailable OC.

Field surveys of sediment-associated OC (and related biogeochemical data) conflicted with priming expectations. We found that inputs of thermodynamically favorable OC protected thermodynamically unfavorable mineral-bound OC. We also found that riparian vegetation shifted biochemical pathways that drive the oxidation of OC. Further, despite the respective oxidation of water-soluble vs. mineral-bound OC pools in dense and sparsely vegetated areas, thermodynamically favorable OC was preferentially depleted in both areas. This suggests universal thermodynamic principles underlie biogeochemical cycling in the hyporheic zone.

In contrast, field surveys of pore water were consistent with priming. Groundwater contained thermodynamically favorable OC at low concentrations while surface water contained thermodynamically unfavorable OC at higher concentrations. As such, OC oxidation was concentration-limited in groundwater and thermodynamically-limited in surface water. When groundwater mixes with surface water, thermodynamically favorable OC in groundwater primes the oxidation of less favorable OC in surface water. We also show concomitant shifts in microbial communities and OC biochemical transformations. These results provide a mechanistic foundation for modeling hyporheic zone biogeochemistry under dynamic mixing.

The contrasting results from sediment-associated vs. pore water OC align with equivocal results in the literature regarding priming effects in aquatic habitats. This highlights the paucity of knowledge related to processes linking OC speciation to hyporheic zone biogeochemical function. Our studies do, however, provide conceptual hypotheses that will be pursued through an iterative model-experiment approach in the next triennial period of the PNNL SFA. Resulting process-based understanding will be used to inform reactive transport models and, ultimately, the development of a process-based watershed modeling framework.

Subsurface Biogeochemical Research

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

Poster #185

ORNL's Critical Interface Science Focus Area (CI-SFA): An Overview

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Developing a process-rich, predictive capability that integrates field, laboratory, and modeling studies of mercury fate and transformation dynamics across broad spatio-temporal scales in low-order streams is the overarching aim of the Critical Interfaces Science Focus Area (CI-SFA) at ORNL. The overarching aim will be accomplished over three successive 3-year phases. The **Phase I** focus is to **determine the fundamental mechanisms and environmental factors that control mercury biogeochemical transformations at key interfaces in terrestrial and aquatic ecosystems.**

Low-order freshwater streams, such as East Fork Poplar Creek (EFPC) (the project's representative use case), constitute nearly 90% of the total stream length in the United States and are the most frequently occurring stream type (>85%). Because of their low hydraulic radius (cross-sectional area and wetted perimeter) and low average water velocity, these stream systems have high water-sediment contact times, which promote in-stream biogeochemical interactions and exchange. Questions being addressed in **Phase I** of the CI-SFA plan include:

- What is the role of EFPC periphyton biofilms in Hg transformations? Which Hg-methylating microbial groups dominate in different EFPC ecosystem compartments?
- What are the key geochemical and biochemical variables and their interactions affecting Hg-DOM complexation, Hg-cell surface interactions, cellular uptake, and methylation?
- How do cell-cell interactions and microbial community metabolism influence net monomethyl mercury (MMHg) production? What is the native function of Hg-methylation gene pair *hgcAB*?
- Which metabolic pathway feeds into reactions involving HgcAB? What are the molecular-scale drivers that control the behavior of Hg-NOM complexation?

Accomplishments in 2016 include a series of recent publications that highlight the role of periphyton biofilms on net monomethyl mercury (MMHg) production in EFPC, the discovery of an iron-reducing bacterium *Geobacter bemidjensis* Bem capable of both methylating Hg and degrading MMeHg, the design of *hgcAB* biomarkers, and first-of-a-kind measurements of Hg-DOM complexes present in EFPC that influence Hg bioavailability. In addition to these publications, new results collected include characterizing HgS aggregates isolated from EFPC soils, delineating the global proteomic profiles of *G. sulfurreducens* PCA after *hgcAB* gene deletion, elucidating the roles of thiol ligands in Hg cellular sorption and bioavailability, applying the *hgcAB* biomarkers to a range of environmental systems (e.g., EFPC and SPRUCE), probing the transformation mechanisms from dimethylmercury to MMHg with DFT, and developing a proto-type simulation tool to predict mercury fate and transformation in low-order streams. Although the CI-SFA uses Hg and EFPC as representative use cases, the information generated and the integrated multi-scale approach can be extended to the understanding of biogeochemical processes that affect fate, toxicity, and fluxes of nutrients and other trace metals and radionuclides in complex, heterogeneous, and multi-scale environmental systems.

Poster #186

Measurement and Modeling of Methylmercury Production in Periphyton Biofilms

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Biogeochemical gradients established across the water – periphyton – stream bed sediment interfaces create zones that can exert controlling influence on material transformations. In this task, we address the role of the water-biofilm interface on mercury (Hg) transformations as a use case. Previous SFA research demonstrates that actively photosynthesizing periphyton biofilms are net sources of the potent neurotoxin monomethyl mercury (MMHg) in East Fork Poplar Creek (EFPC) in Tennessee. Net MMHg production in environmental settings occurs in a broad and complex biogeochemical framework requiring bioavailable Hg, anaerobic conditions, active methylating microorganisms, and methylation rates that exceed those of competing reactions (e.g. demethylation, reactions that sequester Hg). Ancillary chemical analyses of the EFPC biofilms demonstrate active anaerobic communities are present. Microelectrode techniques demonstrate steep gradients in biogeochemical parameters and dynamic Fe and S redox cycling across a few millimeters of the water-biofilm interface. Bulk measurements of periphyton show low molecular thiol compounds that can enhance Hg bioavailability are present in the extracellular matrix.

Periphyton grown on surfaces at upstream (closer to the historic point source of contamination) and downstream locations (~17 km apart) were collected for use in laboratory time-course assays of inorganic Hg methylation and MMHg demethylation. Tin(II) reducible Hg was measured over time as a proxy measure of Hg available for methylation. Additionally, the influence of season and light exposure during biofilm growth were investigated.

The data were divided into a model training data set and validation data set. Methylation (k_m) and demethylation (k_d) rate constants were determined by fitting a series of increasingly complex kinetic models to the training data. Model formulations followed the progression: Model 1: methylation and demethylation were assumed to be irreversible over the incubation time course and each methylation and demethylation data set was modeled in isolation; Model 2: Hg was assumed to cycle between Hg and MMHg during experiments and paired methylation-demethylation rate data were modeled simultaneously; Model 3: same as Model 2 with the added assumption of a time-dependent accumulation of Hg in a pool that is unavailable for methylation.

Both Hg methylation and MMHg demethylation occur within the periphyton biofilms. Upstream versus downstream differences in net methylation were driven by differences in k_d (lower downstream). Within-site temperature-dependent differences in net methylation were driven by changes in k_m (increased with temperature). Compared to samples grown and incubated in the light, samples grown and incubated in the dark had similar k_m values but k_d values that were 10× greater. Models 1 and 2 provided comparable fits to the data and could not capture the observed early time change in methylation rate. Model 3 outperformed Models 1 and 2, and reproduced the early change in the methylation rate. Using parameter estimates from fitting Model 3 to the training data, the validation data set was predicted. Overall, Model 3 approximated the validation data set reasonably well. Assessment of model-prediction uncertainty is ongoing.

Poster #187

Modeling Solute Transport and Coupled Biogeochemical Transformations in Low-order Streams Using a Stochastic Travel-time Approach

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The transport and transformation of carbon, nutrients, and trace metals in low-order streams are controlled to a large degree by contact time with hyporheic and transient surface storage zones that act as local biological “hot spots” for transformation processes. Travel-time based representations provide an alternative to detailed three-dimensional simulations for those multiscale reactive transport processes. In the Lagrangian travel-time conceptualization, computationally demanding three-dimensional reactive transport simulations are replaced with one-dimensional reactive transport simulations on an ensemble of trajectories through the stream channel, transient surface storage zones, and hyporheic zones. The approach is particularly appealing for broad-scope sensitivity analyses. We use mercury as a use case, and consider a simplified model for mercury methylation in low-velocity hyporheic zones and stagnant zones that are diffusively coupled to advective flow paths, accounting for transport of dissolved organic carbon, oxygen, nitrate, sulfate, inorganic mercury, and methylmercury. Growth and decay of biomass is modeled explicitly in low-velocity hyporheic transport pathways, assuming limits on biomass carrying capacity of the sediments and dual-Monod kinetics with phenomenological inhibition functions to suppress activity of nitrate- and sulfate-reducing bacteria when more energetically favorable reactions are possible. Mercury methylation is assumed to be a byproduct of the activity of sulfate-reducing bacteria. The relationships between the travel-time distributions and reach-scale methylation rates are analyzed, addressing both shallow hyporheic flows and horizontal hyporheic flows driven by planimetric variations such as meander bends. Biomass dynamics are not addressed explicitly in the scenarios that consider methylation in biofilms that are diffusively coupled to advective pathways. Instead, the focus is on identifying how that small-scale process manifests at reach scales, specifically how the effect of those small-scale heterogeneities can be represented in reach-scale models by upscaling the reaction inhibition functions.

Poster #188

Elucidating Mechanisms of Natural Dissolved Organic Matter (DOM) in Influencing Mercury Chemical Speciation and Microbial Methylation

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The chemical speciation and bioavailability of mercury (Hg) for methylation are markedly influenced by its redox transformation and complexation with DOM in aquatic environments. However, to date the effects of DOM on Hg complexation, species transformation, and microbial methylation remain obscure, partly due to heterogeneous nature and unknown molecular composition of DOM. In this study, we systematically investigated and compared the effects of DOM on Hg methylation by an iron-reducing bacterium *Geobacter Sulfurreducens* PCA and a sulfate-reducing bacterium *Desulfovibrio desulfuricans* ND132 under anaerobic conditions. We also utilized ultra-high resolution Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) to identify Hg-DOM complexes and to profile DOM compositional changes during photochemical transformation of Hg in water. We demonstrate that DOM effects on microbial methylation are bacterial strain-specific, time- and DOM-concentration dependent. Addition of small amounts of DOM greatly inhibits Hg methylation by *G. Sulfurreducens* PCA but enhances Hg methylation by *D. desulfuricans* ND132 cells in the dark. The result suggests that the effects of DOM on Hg methylation vary due to DOM competitive interactions with microbial cells for Hg uptake and are likely influenced by relative binding affinities of Hg with DOM and microbes. We also found that photochemical reactions of Hg-DOM complexes result in decrease in Hg reactivity and methylmercury production by *G. sulfurreducens* PCA cells. Decrease in Hg reactivity proceeded at a faster rate with a decrease in the Hg to DOM ratio and is attributed to the photolysis of Hg-thiolate complexes in DOM leading to the formation of mercury sulfide (HgS) and loss of S-containing DOM molecules. This observation reveals a potential new pathway of abiotic photochemical formation of HgS in surface water and provides a mechanism whereby freshly deposited Hg is readily methylated but, over time, progressively becomes less available for microbial uptake and methylation. For the first time, we also demonstrate the use of FTICR-MS to unambiguously identify specific DOM molecules in Hg binding. We found that heteroatomic molecules, especially those containing multiple S and N atoms, are among the most important in forming strong complexes with Hg. Major Hg-DOM complexes such as $C_{10}H_{21}N_2S_4Hg^+$ were identified based on both the exact molecular mass and patterns of Hg stable isotope distributions detected by FTICR-MS. Together our results provide new insight into the roles and mechanisms of DOM on Hg chemical and photochemical transformation and its bioavailability leading to the formation of neurotoxic methylmercury in natural aquatic ecosystems.

Poster #189

Application of *hgcAB* Biomarker Detection and Characterization in the Environment

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Methylmercury (MeHg) is a common toxic contaminant but the relationship between the bacteria that produce MeHg and its concentration in the environment is poorly understood. The genes *hgcAB* are essential for microbial mercury (Hg) methylation. We recently developed universal qualitative *hgcAB* as well as quantitative clade-specific *hgcA* PCR probes for the three dominant Hg-methylating clades: *Deltaproteobacteria*, *Firmicutes*, and methanogenic *Archaea*. Here we apply these tools to environmental samples. To link *hgcAB* abundance and diversity with MeHg production, we compared *hgcA* qPCR abundance estimates as well as PCR estimates of diversity to metagenomic shotgun and 16S rRNA amplicon sequencing.

As a preliminary study to ensure the broad applicability, we examined samples from eight Hg-contaminated sites ranging in total Hg (HgT; 0.03-14 mg Hg/kg soil) and MeHg (0.05-27 µg Hg/kg soil) concentrations.

Metagenome and amplicon sequencing revealed that *hgcAB* diversity was dominated by *Deltaproteobacteria* in all eight sites while *Firmicutes* and methanogenic *Archaea* were ~50% less abundant. Results are currently being validated by *hgcA* qPCR. 16S rRNA sequencing did not identify *hgcAB* bacteria well. Overall, PCR-based *hgcAB* methods for Hg-methylator diversity are tractable for studying the relationship between Hg-methylators and soil Hg concentrations at a much reduced cost as compared to metagenomics.

We applied our *hgcAB* and *hgcA* biomarker tools to geochemically variable samples to ensure broad applicability. First, using anaerobic estuarine sediment slurry incubations from salt-marsh soils amended with isotopically labeled complexes of inorganic Hg, we confirmed the presence of *hgcAB*⁺ bacteria, with *hgcA*+ *Deltaproteobacteria* being predominant. Second, using soil cores from the Spruce-Peatland Response Under Climate and Environmental Change (SPRUCE) experiment, we confirmed the presence of *hgcAB*⁺ bacteria in all samples. Sequencing of *hgcAB* amplicons is currently underway to ascertain the Hg-methylator diversity. Lastly, we are currently using our PCR and qPCR *hgcA(B)* biomarker tools to analyze ~50 filters obtained from the oxygen-minimum zone of the Atlantic Ocean during a longitudinal cruise study from Iceland to Brazil. During these studies we have found that optimization for DNA extraction is usually required and is dependent upon the organic matter component of each environmental sample.

Poster #190

Assessment of Microbial Community Responses Towards a Model Synthetic Community for Studying Multispecies Hg-methylation

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Neurotoxic methylmercury (MeHg) is produced by anaerobic bacteria possessing the genes *hgcAB*. The native *hgcAB* function is undetermined so it is unknown which if any carbon or electron sources may stimulate or hinder Hg-methylation. Several carbon sources were amended to East Fork Poplar Creek sediments and a background site to determine their effect on net Hg-methylation. Sediments were assessed for Hg and MeHg levels post-incubation as well as overall microbial diversity via 16S rRNA sequencing and Hg-methylating clade abundance via *hgcA* qPCR. Minimal increases in MeHg were observed with lactate, ethanol and methanol while a significant decrease (~70%) was observed with cellobiose in downstream EFPC. Sequencing revealed that unamended sediments consisted of Proteobacteria, Firmicutes, Bacteroidetes and Actinobacteria with *hgcAB*-containing Bacteria and Archaea identified across all sites. Cellobiose shifted the communities to ~90% non-*hgcAB* containing Firmicutes (mainly *Bacilli spp.* and *Clostridium spp.*) and were verified with *hgcA* clade-specific qPCR analysis. These results suggest that either expression of *hgcAB* is down-regulated or, more likely given the lack of 16S rRNA presence after cellobiose incubation, Hg-methylating organisms are largely incapable of surviving on cellobiose or its degradation products.

In an inter-task effort (see Brooks poster), we have been enriching sulfate- and Fe(III)- reducing bacteria as well as methanogens from East Fork Poplar Creek periphyton. These isolates will be used to construct a Hg-methylating model synthetic community to determine the effect of geochemical and other perturbations on net MeHg production.

We will take advantage of the carbon information and the effect on net MeHg production for use in our model communities. Finally, both in isolation and in the synthetic communities, we will utilize a new TNLEseq capability that will allow for determining the fitness of most genes in each community member species. This may also allow for the elucidation of the essential genes and biochemical pathways required for *hgcAB* functionality.

Poster #191

Biomolecular Insights into the Transport and Transformations of Mercury

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The natural biogeochemical cycling of highly mobile, bioavailable and extremely neurotoxic methylmercury significantly elevates the ecological and public health risk of environmental mercury (Hg). The mechanisms by which microorganisms take up inorganic Hg^{II} substrates and export CH₃Hg-containing molecular species remain unclear. As a first step in understanding microbial Hg uptake/export, we assess the plausibility of passive diffusion of neutral Hg^{II} *bis* thiolate and CH₃Hg-thiolate complexes across a model microbial cytoplasmic membrane in the absence of membrane proteins. Through extensive molecular dynamics simulations, we quantify the energetics of passive diffusion and show that it is energetically feasible for neutral Hg-containing species.

In other work, we have used density functional theory (DFT) to investigate mechanisms of the formation of dimethylmercury from monomethylmercury mediated by reduced sulfur-containing compounds. The calculations reveal chemical trends in Hg–C bond strengths under different thiolate coordination environments and show how the stabilization of Hg permits methyl ligand exchange to a more electrophilic partner. Furthermore, we show that two adjacent [CH₃Hg]⁺–thiolate complexes form an unusual dinuclear Hg^{II} complex that serves to accomplish maximal Hg stabilization during the transmethylation reaction. These findings are rationalized within the context of our previous work on the mechanisms of demethylation of methylmercury by MerB and the methylation of inorganic Hg^{II} by HgcA. Together, these studies demonstrate the unique ability of computation to reveal important physicochemical insights while circumventing the handling of hazardous materials.

Poster #192

The Biochemistry of Mercury Methylation in Anaerobic Bacteria

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Microbial mercury methylation is an enzyme-catalyzed process carried out by certain anaerobic bacteria and archaea. The two-gene cluster *hgcAB* is essential for mercury methylation and encodes a cobalamin-dependent protein, HgcA, and a ferredoxin, HgcB, which are predicted to facilitate methyl transfer and cofactor reduction, respectively. Determining the specific roles and interactions of HgcA and HgcB with other cellular components offers insights into the biochemical pathways associated with bacterial mercury methylation. The results will help reveal key processes that control the fate and transformation of mercury in freshwater ecosystems and will provide essential data to inform metabolic and reactive transport models that can be used to predict mercury cycling from the molecular to the field scale.

The goal of this work is to identify molecular mechanisms and interactions of HgcA and HgcB to elucidate the biochemistry of mercury methylation. Heterologous expression of HgcB in *E. coli* as an N-terminal maltose-binding protein fusion in *E. coli* BL21(DE3) resulted in purified HgcB, which is 65% replete with [4Fe-4S] clusters. UV-Vis spectroscopic data demonstrates electron transfer to HgcB *in vitro* and the interaction of HgcB with Hg(II) has been characterized. Furthermore, *Desulfovibrio desulfuricans* ND132 strains were engineered for tandem affinity purification of HgcA and HgcB with 3xFLAG/TEV/StrepII tags in order to overcome limitations resulting from low abundance of the native proteins in cells. ND132 strains expressing tagged HgcA or HgcB retain mercury methylation activity at >50% of the wild-type strain. Preliminary results from tandem affinity purification and immunoblotting indicate that native HgcB can be purified to homogeneity pending verification by mass spectrometry. Ongoing work aims to develop a protocol to isolate native HgcA at sufficient yields for spectroscopic characterization. Covalent crosslinking will be used to reveal protein-protein interactions, which will in combination with structural bioinformatics help delineate the roles of HgcA and HgcB in the context of microbial carbon metabolism. A comprehensive understanding of the various geochemical and biochemical factors culminating in the production of MeHg will facilitate the development of effective strategies to limit production and bioaccumulation of methylmercury in the environment.

Subsurface Biogeochemical Research

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

Poster #204

LLNL Scientific Focus Area – Subsurface Biogeochemistry of Actinides

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The objective of LLNL's SFA is to *identify and quantify the biogeochemical processes that control the fate and transport of actinides in the environment*. The research approach combines three Thrusts: (1) **Fundamental Mechanistic Studies** that identify and quantify biogeochemical processes, (2) **Field Integration Studies** that investigate the transport characteristics of Pu in the environment, and (3) **Actinide Research Capabilities** that provide new opportunities for advancing actinide environmental chemistry.

Research Thrusts 1 and 2 are guided by broad central hypotheses:

***Thrust 1 Hypothesis:** The biogeochemical mechanisms controlling **redox transformations of actinides and their stabilization** as aqueous complexes, binary surface complexes, ternary surface complexes, precipitates, and co-precipitates will determine actinide migration in the environment.*

***Thrust 2 Hypothesis:** The biogeochemical processes that ultimately control actinide subsurface mobility/immobility are driven by local variations in the geology, geochemical conditions, colloid composition and abundance, and **chemical characteristics of the initial actinide source**.*

Research Thrust 3 is not hypothesis driven. Instead, it is guided by the research efforts and capability development needs described in Research Thrusts 1 and 2.

Here, we summarize the accomplishments from 2016 that span all three Thrusts. Pu(IV) and Pu(V) sorption to goethite at sub-femtomolar to micromolar concentrations revealed how concentration affects redox transformation rates and formation of surface precipitates. The effect of natural organic matter on Pu sorption to goethite was examined to identify solution conditions that lead to formation of ternary surface complexes. The interactions of Pu with *Pseudomonas* sp. Strain EPS-1W and its extracellular polymeric substances was investigated to determine the role of microbes in Pu transport. Desorption rates of plutonium from montmorillonite colloids was investigated to determine the extent of colloid-facilitated transport at environmentally relevant timescales. Colloid-facilitated transport experiments of Th(IV) with hematite ($\alpha\text{-Fe}_2\text{O}_3$) colloids and Suwannee River fulvic acid were performed to examine ternary colloid transport rates. Long-term (~6 year) diffusion of U(VI) through bentonite was investigated and revealed much slower migration behavior than observed in short-term experiments. The pressure dependence of carbonate exchange with $[\text{NpO}_2(\text{CO}_3)_3]^{4-}$ in aqueous solutions was studied to quantify molecular scale rate-limiting processes and revealed that f-electrons affect ligand exchange mechanisms and rates. A novel solid-state NMR method for the investigation of trivalent lanthanide sorption on amorphous silica at low surface loadings was developed for use in actinide mineral-water interface studies. Finally, a review paper entitled "Behavior of plutonium in the environment" was published together with our Russian collaborators in a special issue of Russian Chemical Reviews devoted to the Boris Myasoedov 85th anniversary. This work was supported by the Subsurface Biogeochemical Research Program of the U.S. Department of Energy's Office of Biological and Environmental Research.

Poster #205

Characterization of Redox Mediated Alterations in $\text{PuO}_2(\text{s})$, $\text{NH}_4\text{PuO}_2\text{CO}_3(\text{s})$ and $\text{NpO}_2(\text{s})$ Sources in Multi-Year Field Lysimeter Studies

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The RadFLEx (Radionuclide Field Lysimeter Experiment) at the DOE Savannah River Site is examining long-term vadose zone transport of Np and Pu under natural conditions. In this experiment, $\text{Pu}(\text{IV})\text{O}_2$, $\text{Np}(\text{IV})\text{O}_2$, $\text{Np}(\text{V})\text{O}_2\text{NO}_3$, and $\text{NH}_4\text{Pu}(\text{V})\text{O}_2\text{CO}_3$ sources (as 1-10 mg solids sandwiched between glass fiber filter papers) are buried midway in a sandy clay loam soil filled 61 cm long x 10 cm diameter lysimeters. Pu lysimeters were deployed in triplicate and Np lysimeters in duplicate for multi-year retrieval and analysis. Additionally, a set of archived sources were preserved in the laboratory under inert conditions. Leachate is collected from these lysimeters approximately every three months to provide a measure of radionuclide transport.

Comparison with data from previous field lysimeter experiments with plutonium originating from $\text{Pu}(\text{VI})$ sources was transported significantly further than $\text{Pu}(\text{IV})$ sources. New experiments with a soluble $\text{NH}_4\text{Pu}(\text{V})\text{O}_2\text{CO}_3$ source indicated relatively little transport of Pu after 2.5 years with greater than 95% of the plutonium remaining within the source. X-ray absorption spectroscopy (XAS) analysis of initial source archived in an inert atmosphere and sources exposed to lysimeters indicate some reduction to $\text{Pu}(\text{IV})$ within the sources leading to the formation of $\text{Pu}(\text{IV})\text{O}_2$. Thus, there appears to be an auto-reduction of $\text{NH}_4\text{Pu}(\text{V})\text{CO}_3$ to $\text{Pu}(\text{IV})\text{O}_2$ even under inert conditions. However, solvent extraction on archived and field-deployed sources show the archived source still contains around 40% $\text{Pu}(\text{V})$ whereas the same source from a field lysimeter deployed for 2.5 years contained less than 10% of $\text{Pu}(\text{V})$. Laboratory studies have shown that the presence of sediment accelerates the reduction of $\text{Pu}(\text{V})$ to $\text{Pu}(\text{IV})$.

A second set of lysimeters contain $\text{Np}(\text{IV})\text{O}_2$ and $\text{Np}(\text{V})\text{O}_2\text{NO}_3$ sources for comparison with the Pu sources. Aqueous Np was measured in the effluent from duplicate $\text{Np}(\text{V})\text{O}_2\text{NO}_3$ bearing lysimeters within 18 months of deployment whereas Np was not measured in the effluent of initially $\text{Np}(\text{IV})\text{O}_2$ lysimeters for 4 years. After recovery of one $\text{Np}(\text{V})$ and one $\text{Np}(\text{IV})$ source after 4 years of exposure, more than 99% of the total Np was leached from the initially $\text{Np}(\text{V})\text{O}_2\text{NO}_3$ source and approximately 50% was leached from the initially $\text{Np}(\text{IV})\text{O}_2$ source. Transport from the $\text{Np}(\text{IV})\text{O}_2$ source was not expected due to the low solubility of source material. However, as this was observed, it is likely that the source has oxidized from $\text{Np}(\text{IV})$ to $\text{Np}(\text{V})$ while in contact with oxidizing rainwater. The concentrations of Np in the soil from the $\text{Np}(\text{IV})\text{O}_2$ source are an order of magnitude lower than in the $\text{Np}(\text{V})\text{O}_2\text{NO}_3$ source, suggesting that the entirety of the source has not oxidized. Electron microscopy and x-ray absorption spectroscopy (XANES/EXAFS) analysis of the source materials have verified oxidation of $\text{Np}(\text{IV})$ to $\text{Np}(\text{V})$ as well as a shift from a crystalline to an amorphous phase. Our current efforts are relating these observed changes in source oxidation state to the migration of Pu and Np within the lysimeters.

This work was supported by the Subsurface Biogeochemical Research Program of the U.S. Department of Energy's Office of Biological and Environmental Research.

Poster #206

Pu(VI) Hydroxamate Complex Formation at Circumneutral pH

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Plutonium represents a major environmental and public health concern due to its long half-life ($t_{1/2} \sim 24000$ yrs.), toxicity and ability to migrate (kilometers) in the environment. Understanding the fate of radionuclides in the environment requires knowledge of the fundamental biogeochemical processes that control actinide speciation, precipitation and transport. One such example is the ability of microorganisms to react with Pu through surface adsorption, redox or the secretion of chelating agents. Siderophores are produced by microorganisms and plants to chelate insoluble Fe(III), making it available for cellular uptake. Siderophores with hydroxamate functional groups also form strong pH dependent complexes with Pu(IV), influencing Pu transport in the environment. The degradation of siderophores leads to the release of simple mono- and di-hydroxamates with somewhat lower metal affinities. Interestingly, these types of simple hydroxamates (acetohydroxamic acid, AHA) have been used in nuclear fuel processing due to their ability to selectively reduce Np(VI) and Pu(VI) in the presence of nitric acid (1-4M). These studies suggest that Pu(VI) reduction to Pu(IV) occurs by a rapid electron exchange with AHA followed by slow continued reduction by AHA acid hydrolysis products (hydroxyl amine). By analogy, it has been suspected that hydroxamate moieties may reduce Pu(VI) to Pu(IV) under environmentally relevant solution conditions at circumneutral pH as well. However, the reactions of Pu(VI) with AHA at environmentally relevant pH (6-8) have not been reported in the literature. We measured the reactions of Pu(VI) with varying concentrations of AHA at circumneutral pH using UV-Vis-NIR spectroscopy to track the reduction of Pu(VI) (absorption band at 831nm) and GC-MS to measure the breakdown of AHA to hydroxylamine. Our results show that Pu(VI) forms a stable complex with AHA at pH 6-8, which results in the loss of the Pu(VI) peak at 831nm. The concentrations of AHA remained constant and no production of hydroxylamine occurred, suggesting that the loss of the Pu(VI) absorption peak occurred due to ligand formation rather than reduction to Pu(IV). Subsequent acidification (0.5M HNO₃) caused dissociation of the of the Pu(VI)-AHA ligand complex and the reappearance of the free Pu(VI) peak at 831nm. These results suggest that Pu(VI) will form a stable complex with AHA, at environmental pH, that does not result in the reduction of Pu(VI) to Pu(IV).

Poster #207

Plutonium Incorporation into Iron Oxide Minerals

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For the long-term performance assessment of nuclear waste repositories, knowledge about the interactions of actinide ions with mineral surfaces is imperative. In the United States, nuclear weapons production and testing has led to approximately 10^{14} Bq of ^{239}Pu subsurface contamination at the Hanford site and more than 10^{15} Bq of plutonium contamination at the Nevada National Security Site (previously Nevada Test Site). Plutonium is a highly toxic, long lived radionuclide characterized by complex chemical and physical properties and much attention has been paid to understanding its behavior in order to guarantee safe handling and long term storage. The mobility of plutonium (Pu) in the subsurface is affected by Pu-mineral interactions such as adsorption-desorption and structural incorporation. Previous studies have demonstrated a high affinity of Pu for Fe-oxide minerals that are ubiquitous in the environment and are characterized by high redox reactivity and surface area. In addition to forming in soil and sediments, iron (oxy)hydroxides form as corrosion products of steel and are present in intermediate level of radioactive waste. The hydrous ferric oxide, ferrihydrite, is a common, poorly crystalline, metastable early product of both biotic and abiotic precipitation of iron, and is a precursor to other more crystalline iron oxides such as hematite (Fe_2O_3) and goethite (FeOOH). It has been shown that goethite and hematite are able to accommodate various impurities into their structure including Si, Ti, Mn, Ni and U(VI). The aim of this work is to evaluate how Fe-oxide minerals structurally incorporate plutonium during crystallization. By studying various synthetic iron oxides co-precipitated with Pu(IV) we are aiming at determining the mechanism of plutonium incorporation and define the atomic scale bonding environment of Pu in the various mineral structure. Ferrihydrite, goethite and hematite have been synthesized from solution with varying amount of plutonium (100s-1000s of ppm). The extent of Pu incorporation into ferrihydrite and subsequent alteration to goethite and hematite was monitored by liquid scintillation counting. Mineral powders were characterized by P-XRD, SEM, and HR-TEM. Preliminary data indicate that sorption equilibrium of Pu(IV) onto ferrihydrite is reached within one week. Upon transformation of Pu(IV)-ferrihydrite, goethite showed a higher extent of Pu-incorporation than hematite. The extent of Pu incorporation in ferrihydrite, goethite and hematite has important implications for the long-term performance of nuclear waste repositories, particularly from the standpoint of irreversible association of Pu with mineral phases.

Subsurface Biogeochemical Research

**Argonne National Laboratory
SBR Science Focus Area**

Poster #211

The Argonne National Laboratory Subsurface Biogeochemical Research Program SFA: Fe and S Biogeochemistry in Redox Dynamic Environments

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Understanding the interplay of the Fe and S biogeochemical cycles with the hydrologic cycle is essential to accurately predict atmospheric greenhouse gas emissions; carbon cycling and sequestration in subsurface environments; nutrient mobility; and the mobility of contaminants in near-surface and subsurface polar, temperate, or tropical systems. The objective of the Argonne Subsurface Biogeochemical Research Program (SBR) Scientific Focus Area (SFA) is to identify and understand the coupled biotic-abiotic transformations of Fe and S within redox-dynamic environments at the molecular- to core-scale, as well as to understand the effects of Fe and S biogeochemistry on the transformation and mobility of major/minor elements and contaminants. To accomplish this objective, the Argonne SBR SFA integrates two key analytical strengths at Argonne — the Advanced Photon Source (APS) for synchrotron-based interrogation of systems and next-generation DNA sequencing and bioinformatics approaches for microbial community and metabolic pathway analysis — with biogeochemistry and microbial ecology. Addressing this objective contributes directly to the goal of the United States Department of Energy (DOE), Office of Biological and Environmental Research (BER), Climate and Environmental Sciences Division (CESD) to “advance fundamental understanding of coupled biogeochemical processes in complex subsurface environments to enable system-level environmental prediction and decision support.”

Argonne SBR SFA research addresses four critical knowledge gaps: (1) an in-depth understanding of the molecular processes affecting Fe, S, and contaminant speciation in dynamic redox environments; (2) an understanding of the role of biogenic and abiotic redoxactive products and intermediates in Fe, S, and contaminant transformations; (3) a mechanistic understanding of the factors controlling the mass transfer of Fe, S, and contaminants in heterogeneous media; and (4) an in-depth understanding of the relationship between microbial community dynamics/function and coupled biotic-abiotic controls, and their effects on major/minor element cycling and contaminant transformations.

The long-term vision of the Argonne SBR SFA envisions ultimately integrating the new mechanistic knowledge generated by the SFA into multiscale Earth system models to enhance their predictive power for relevant environmental processes. The ten year vision also includes (1) an ever-increasing emphasis on integrating omic-based analysis approaches for understanding ecological and functional controls on the biogeochemistry of Fe and S, (2) an increasing emphasis on model development to predict the transformations and mobility of nutrients and contaminants in many subsurface and near-surface environments, and (3) expansion of these studies with a greater emphasis on using minerals and microbial communities from a network of field sites encompassing many types of redox-dynamic environments.

Poster #212

Using X-Ray Spectroscopy to Define the Interplay Between Fe, S, and U Dynamics in Batch Reactors and Flow-Through Columns

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Successful modelling of elemental cycling and contaminant transport in natural environments requires detailed knowledge on the transformations of the major, minor, and contaminant elements. Information such as the reactive species, the products, and the kinetics of transformation is needed for the definition of reactions in Reactive Transport Models (RTMs). While mechanistic information is available for some reactions, others are included empirically and may not reflect the actual mechanism. The disadvantage of not including a reaction or using an incorrect reaction is that the model predictions may become inaccurate outside the conditions where the model was validated.

The Argonne Subsurface SFA is continuing to provide the mechanistic understanding of processes needed for the improvement of RTMs. We have studied the transformations of U in the presence of reduced subsurface components (Fe-containing clays and green rusts, GRs). We used carbonate extractions and XAFS spectroscopy to investigate the identity and stability of the phases resulting from U^{VI} reduction by biogenic and abiotic GRs. The results show that the initial products in the abiotic GR system were U^{IV}-carbonate complexes, which transformed to uraninite over several days. The proportion of extractable U concurrently decreased from ~95% to ~10%. In contrast, the solid-phase U^{IV} atoms in the biogenic GR system remained as non-uraninite U^{IV} species that were labile (~80% extractable).

The role of clays as adsorbents and redox buffers in subsurface environments is recognized but remains poorly understood. Using XAFS spectroscopy we studied the reducibility of Fe^{III} in SWy-2 and NAu-1 clays by sulfide or AH₂QDS. The addition of 0.2 – 10 mM sulfide leads to increasing extents of Fe^{III} reduction in 2g/L SWy-2 clay, without ferrous sulfide formation. The same limiting extent and EXAFS spectrum were observed with 2mM AH₂QDS as the reductant, also indicating lack of ferrous sulfide formation. The role of clays in controlling U speciation was also explored. We find that low loadings of reduced clay minerals reduce U^{VI} to a mixed-valence U^V-U^{VI} oxide, whereas higher loadings result in the formation of uraninite and adsorbed U^{IV} species. By varying the amounts of reductant and surface in the system we find that the stabilization of the U^V or U^{IV} state is controlled by the reducing capacity, whereas the distribution between uraninite and adsorbed U^{IV} is controlled by surface site availability. These reaction pathways are currently not included in transport models, but may be important in governing U transport in sediments with fluctuating reducing conditions.

Poster #213

Electron Shuttle Effects on Iron(III) Reduction, Methane Production, and Microbial Community Dynamics

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Dissimilatory metal-reducing bacteria (DMRB) gain energy by coupling the oxidation of reduced organic compounds or H₂ to the reduction of iron and other metal oxides. These oxides are poorly soluble at the temperature and pH ranges typical of most subsurface environments, and consequently many DMRB use soluble electron-shuttling compounds to aid the extracellular transfer of electrons to these electron acceptors. Pure culture studies suggest these shuttles enhance the overall rate of iron reduction, yet little is known about how the presence of these compounds affects complex native communities of microorganisms under iron-reducing conditions. Using wetland sediment microcosms amended with goethite (α -FeOOH) and either acetate or H₂, we examined the effect(s) that individual quinone-based electron shuttles with differing redox potentials have on the rate of iron reduction, the time-to-onset of methanogenesis, and the trajectory of microbial community development. We found the effects of electron shuttles on Fe(III) reduction and methanogenesis were compound specific. 5-hydroxy-1,4-naphthoquinone (lawsone, or NQL) and 1,2-dihydroxy-9,10-anthraquinone (AQZ) had a minimal effect on Fe(III) reduction and methanogenesis relative to the no shuttle (NS) control, while the presence of 9,10-anthraquinone-2,6-disulfonate (AQDS) and 9,10-anthraquinone-2-sulfonate (AQS) led to more rapid Fe(III) reduction and an earlier onset of methanogenesis. Systems amended with 9,10-anthraquinone-2-carboxylic acid (AQC) showed an initially slower rate of Fe(III) reduction and complete inhibition of methanogenesis despite the availability of excess electron donor. Previous work under axenic conditions (*Shewanella putrefaciens* CN32) had indicated a robust relationship between the reduction potential of an electron shuttle and the rate of Fe(II) production, such that AQC>AQS>AQDS>AQZ>NQL>NS. However, in these wetland sediment microcosms, AQDS>AQS>NS≈AQZ≈NQL>AQC, suggesting that the reduction potential is not an effective predictor of the effectiveness of a putative electron shuttle in systems with a diverse microbial community. Members of the *Geobacteraceae* and *Desulfuromonadaceae* dominated in the absence of added electron shuttles and in the presence of AQZ. The *Geobacteraceae* alone dominated NQL- and AQS-amended systems, but were of lower relative abundance in the presence of AQC, in which case *Pelobacteraceae* (acetate-amended) or *Shewanellaceae* (H₂-amended) were dominant depending on the electron donor present. It is not yet clear if AQC acts by directly promoting these taxa, although enrichment of *Geobacteraceae* in one of the three acetate-amended enrichments suggest that they are not specifically inhibited by AQC. The complete inhibition of methanogenesis by AQC highlights the possibility for electron shuttles to influence microbial processes in addition to those involving respiration with insoluble terminal electron acceptors.

Poster #214

Biogeochemical Impacts of the Microbially-Mediated Cycling of Iron and Sulfur

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Microorganisms in the subsurface respire using a variety of terminal electronacceptors, and the resultant geochemical transformations are critical steps in the biogeochemical regulation of these environments. Of these organisms, two of the most important groups are dissimilatory metal-reducing bacteria (DMRB) and sulfate-reducing bacteria (SRB). Through their metabolism, these organisms directly affect the geochemistry of the subsurface through the dissolution of ferric minerals, the consumption of sulfate by SRB, and the subsequent production of reactive ferrous iron and sulfide species. The extent to which either group is active, however, depends upon the geochemical conditions of the particular subsurface environment, such as the pH, temperature, or salinity of the groundwater. In bioreactor experiments of wetland sediment amended with ferric iron minerals, sulfate, and acetate conducted at pH 6 and pH 7.5, we found that pH had a larger influence than acetate concentration on controlling the flux of electrons through iron reduction and sulfate reduction. Under acidic conditions, the amount of iron reduced was a factor of three greater than the amount of sulfate reduced in reactors receiving little (0.25 mM) or no acetate compared to a factor of two in reactors receiving 1 mM acetate. Under alkaline conditions, iron and sulfate were reduced in nearly equal proportions regardless of influent acetate concentration. Results from sulfate-deficient control reactors show that the presence of sulfate reduction increased the extent of iron reduction in all experiments, but particularly in alkaline reactors. Under acidic conditions, the extent of iron reduction was greater by a factor of 1.2 if sulfate reduction occurred simultaneously than if it did not. Under alkaline conditions, that factor increased to 8.2. Hence, pH influenced the extent to which sulfate reduction promoted iron reduction. We also conducted similar experiments employing a newly isolated DMRB from the deep subsurface, *Orenia metallireducens* strain Z6, which can reduce crystalline ferric minerals like goethite and hematite. In similar bioreactors, we examined the effects of a number of environmental factors (pH, temperature, salinity, anion concentration, and availability of electron shuttles) on the bioreduction of a suite of ferric iron minerals (ferrihydrite, lepidocrocite, goethite, hematite, and magnetite). We found that the chemistry of the environment controls not only the rate of microbial iron reduction, but the formation of secondary iron minerals. These controlled laboratory experiments inform ongoing efforts to examine iron and sulfur cycling in redox dynamic environments like wetlands.

Subsurface Biogeochemical Research

SLAC

SBR Science Focus Area

Poster #198

Coupled Cycling of Organic Matter, Uranium, and Biogeochemical Critical Elements in Subsurface Systems. Overview of the SLAC SFA

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Research performed by our group over the past 3 years has shown that organic-enriched sediments are common in shallow sand-pebble-cobble alluvial aquifers in the upper Colorado River Basin (CRB). Organic-enriched bodies are generally sulfidic and referred to as, 'naturally reduced zones' (NRZs), and host large inventories of biogeochemically critical elements and contaminants, including Fe, C, S, N, P, U, Mo, and V. NRZs frequently reside within the capillary fringe where they are exposed to seasonal wet-dry cycling, creating conditions conducive to redox-driven nutrient and contaminant mobilization, with important implications for groundwater quality. Uranium-enriched NRZs are spatially coincident with persistent uranium groundwater plumes, raising the likelihood that sediment-uranium interactions contribute to the longevity of these contaminant hot spots. Seasonal hydrologic variability and organic content are characteristic of floodplains worldwide, and alluvial redox cycling is globally important to water quality. In spite of its importance, there are numerous gaps in our understanding of these hydro-biogeochemically active systems.

We are investigating the fundamental hydro-biogeochemical mechanisms by which NRZs mediate the speciation, behavior, and fluxes of carbon, uranium, and other elements across a range of scales, from molecular to regional. Our goal is to identify, interrogate, and model key processes in shallow alluvial aquifers to improve our understanding of water quality and to support SBR computational capabilities. Questions being investigated include: (i) What are the dominant reactions that occur when NRZs undergo redox transitions?; (ii) What biological, kinetic, and thermodynamic factors control the speciation and behavior of uranium?; (iii) Does microbial N cycling mediate uranium mobilization?; and (iv) How do spatial constraints imposed on metal reducing microorganisms by the insolubility of TEAs influence microbial syntrophy and uranium reduction in NRZs?

We have conducted field-scale investigations at sites across the upper CRB and performed laboratory-based molecular scale investigations using x-ray absorption spectroscopy, x-ray, electron, and isotope imaging, gene sequencing, electrochemistry, and stable isotope techniques. Major scientific contributions over the past year include publication of new process models to describe iron and sulfur cycling in NRZs and their impact on U mobility, a new biogeochemical model for U(IV) behavior in organic-enriched sediments, which is dominated by adsorption to particulate organic carbon, and a new mechanism for organic carbon preservation in anoxic sediments. These findings advance the SBR mission by providing new knowledge about biogeochemical controls over water quality and by providing insights and biogeochemical process representations needed to model contaminant and nutrient behavior.

Poster #199

Redox Constraints on Shallow Alluvial Sediments: Implications for U Mobility

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Redox processes are important mediators of nutrient and contaminant storage and release in alluvial aquifers. Our previous studies show that organic-enriched zones are common in sand-pebble-cobble aquifers in the upper Colorado River Basin (CRB) and develop reducing conditions and sulfidic mineralogy. We refer to these as “Naturally reduced zones” (NRZs). Large inventories of uranium accumulate in NRZs located within persistent uranium groundwater plumes, raising the likelihood that sediment-uranium interactions help to sustain these contaminant hot-spots. The susceptibility of accumulated U(IV) to oxidation and remobilization creates the need to better understand and predict U speciation, the biogeochemical controls on redox conditions in NRZs, and their impact on U storage and remobilization.

In this study, we tracked Fe and S speciation in NRZs as a function of depth, organic carbon content, and grain size in order to better define the biogeochemical controls over the distribution and reactivity of redox process in the upper CRB floodplain sediments. Redox reactivity was then compared with the distribution of U species in order to elucidate factors controlling their stability. We hypothesized that U(IV) in NRZs would be bound to particulate organic matter. In this case, the ability of sediment to stabilize U(IV) would depend on the ability of sediments to physically and chemically protect U from oxidation. Here we show that organic carbon content and moisture are critical factors in the stability of U(IV) in NRZs. Coarse-grained textures allow greater exposure of NRZs to oxidants and conversion of U(IV) to U(VI). We also show that fine-grained NRZs can retain U(VI) produced by oxidation of U(IV) by adsorption on surfaces of solid phases. Finally, our data suggest that, even in the absence of oxidative perturbations, U can be mobilized. Knowledge produced by this work will help to develop conceptual and numerical models of the biogeochemical controls over U transport within alluvial aquifers and provides insights into the mobility of nutrients and other contaminants.

Poster #200

Effects of Microbial Communities on Uranium Oxidation and Mobilization in the Presence of Nitrate, Nitrite, and Oxygen

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Throughout the upper Colorado River Basin, uranium (U) persists as a legacy contaminant of former ore processing activities. Elevated solid-phase uranium levels exist in fine-grained, organic-enriched sediments. Coupled with seasonal groundwater fluctuations that alter the subsurface redox conditions, recent evidence suggests that release of uranium may be controlled by biologically-produced nitrite and nitrate. Previous researchers have posited that nitrate and nitrite can oxidize U(IV). We hypothesize that when seasonal groundwater levels recede and the subsurface system becomes anoxic, nitrate/nitrite diffuses into the reduced interiors of organic-rich sediments and becomes readily available for denitrification, the stepwise anaerobic reduction of nitrate/nitrite to dinitrogen gas. Denitrification may then be coupled to the oxidation of sediment-bound U(IV), forming mobile U(VI) that can be released to the aquifer. Although both abiotic and biotic uranium oxidation have been documented, the rate of uranium oxidation coupled to bacterial nitrate reduction far exceeds observed abiotic oxidation rates. Thus, nitrogen-cycling microbial communities, specifically those involved in denitrification, may be key to understanding uranium mobility and long-standing environmental contamination. However, a paucity of knowledge exists regarding denitrifying communities in the subsurface.

Here we investigate how the indigenous microbial community from fine-grained, organic-enriched sediments responds to an oxidation event. Using flow-through column reactors packed with sterilized or unsterilized organic-enriched fine-grained sediment from a uranium plume at Riverton, WY, we simulated a laboratory-scale oxidation event by stimulating the columns with an oxidant (either 1mM nitrate, 100 μ M nitrite, or 268 μ M oxygen) for 24 days. The objectives of this study were to (1) identify how the type of oxidant introduced affects the denitrifying microbial community from Riverton, WY, and (2) assess over what timescales and to what extent do nitrate, nitrite, and oxygen oxidize uranium in reduced sediments. Preliminary uranium effluent data suggests that uranium mobilization occurred within the first five days and was greatest in the oxygen-stimulated columns. Uranium speciation results show that oxidation proceeded near the influent in the nitrite- [U(VI): 42%] and nitrate- [U(VI): 18%] amended columns; however, in the oxygen-amended columns uranium oxidation was greater [U(VI): 77-82%] and occurred throughout the entire column. These results indicate that oxygen was the most efficient oxidant of uranium within this system and although, the nitrate- and nitrite-amended columns resulted in changes in microbial diversity and abundance, less uranium oxidation and mobilization was observed.

Poster #201

Spatial Constraints on Microbial Metabolic Activity in Anaerobic Environments

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Spatial separation of metabolic substrates creates constraints for microorganisms in any soil environment, but is particularly relevant to microbial metabolic activity in anaerobic sediments. Insoluble particulate organic carbon and mineral bound terminal electron acceptors (TEAs), such as Fe(III) or U(VI), are often not homogeneously distributed, creating a spatial dilemma for metal reducers to physically access both the carbon substrate and TEAs. In naturally reduced zones (NRZs), the reductive immobilization of uranium is closely linked to the gradual degradation of organic matter carried out by consortia of different microorganisms. To evaluate the impact of spatial constraints on microbial syntrophy and metal/uranium fate in NRZs, we have developed a co-culture system with three bacteria representing key metabolic processes: *Ruminiclostridium cellulolyticum* (hydrolysis and fermentation of cellulose), *Geobacter sulfurreducens* (metal reduction), and *Desulfovibrio vulgaris* (sulfate reduction). This co-culture is grown in an electrochemical reactor system where both the carbon source (cellulose) and the fluorine-doped tin oxide (FTO) anode serving as TEA for *G. sulfurreducens*, are immobilized in spatially separated patterns at micro- to millimeter scale. With cellulose as the sole carbon source, both *G. sulfurreducens* and *D. vulgaris* are relying on fermentation products provided by *R. cellulolyticum* for growth. Increasing separation distances between carbon substrate and TEA put *G. sulfurreducens*, who is relying on an immobilized TEA, at an increasing disadvantage compared to *D. vulgaris*, who is using a soluble TEA (sulfate in the medium) and thus can position themselves close to the carbon source. By growing our bacterial model community on spatially patterned glass slides, we are able to microscopically visualize the spatial organization of the community with high resolution and precisely monitor the flow of electrons and carbon through the microbial community. Our experiments will help evaluate the biogeochemical relevance of spatial separation of different metabolic substrates, a constraint imposed on microbial function within NRZs (and other anaerobic environments). Such information is needed to understand the fate of carbon, sulfur, iron, uranium and other metals in NRZs and guide the development of spatially explicit reactive transport models.

Poster #202

Hydrologically Driven Process Coupling Between Biogeochemical Cycles and Solute Transport in Transiently Saturated Sediments at the Riverton Site (WY)

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Water quality in shallow alluvial aquifers is strongly impacted by solute exchange with overlying capillary fringe sediments during seasonal and synoptic water table excursions. During the past three years, we have cored sediments at floodplain sites exhibiting persistent groundwater U plumes within the upper Colorado River Basin. Our examinations of the biogeochemical interactions between sediments and groundwater have indicated the importance of organic matter concentration and sediment texture for governing the retention of U in naturally reduced zones (NRZs) through microbially mediated reduction of U, Fe and sulfate, coupled to organic C oxidation and organic matter complexation. Importantly, our observations imply that the persistence or transiency of reducing conditions is a key regulator of U, Fe, S, and C chemical speciation and reactivity, and governs the partitioning of elements between immobile (solid) and mobile (soluble, colloidal) phases. These observations have focused our attention within the new SLAC SFA science plan on the coupling of hydrological conditions (saturation state and transport mechanisms/directions/rates) to biogeochemical cycles that govern contaminant and nutrient mobility in floodplains.

The U-impacted Riverton (WY) site serves as a model floodplain to investigate the impacts of hydrologically driven biogeochemical processes on groundwater chemistry and quality. Here, we have observed strong reversal in the vertical transport of U in response to spring flooding (downward transport and release to groundwater) and summer drought (evapotranspiration-driven upward transport and precipitation with evaporite minerals). Further, we have observed strong redox cycling of Fe, S, and U in sediments in response to saturation, resulting in U alternately partitioning into solution (oxidized conditions) and onto the solid phase (reducing conditions). Thus, a conceptual model emerges, where hydrologically-initiated biogeochemical redox transformations drive a seasonal cycle of U shuttling vertically with water movement and between different solid phase hosts (evaporite minerals, redox minerals, clays, and organics), pore water, and groundwater. The timing, thresholding conditions, and relative rates of processes are key pieces of information required to mechanistically link hydrological and biogeochemical processes in order to predict U mobility. Our future work at the Riverton site will examine the microbial community composition and activity, pore- and groundwater chemistry, sediment mineralogy, and organic matter composition at molecular to mm scales as a function of depth and time in relation to water saturation and transport mechanisms. Here, we will present preliminary results from exploratory investigations of these aspects within the capillary fringe and plans for future research at the Riverton floodplain.

Subsurface Biogeochemical Research

Interoperable Design of Extreme-Scale Application Software (IDEAS) Project

Poster #215

Interoperable Design of Extreme-scale Application Software (IDEAS): Improving Developer Productivity and Software Sustainability

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While emerging extreme-scale computers provide unprecedented resources for scientific discovery, the community faces daunting productivity challenges due to the complexities of multiphysics, multiscale applications and evolving computer architectures. The IDEAS Scientific Software Productivity Project (<https://ideas-productivity.org>) is working to improve the productivity of software developers and the sustainability of software artifacts—through an interdisciplinary and agile approach that centers on adapting modern software engineering tools, practices, and processes to build a flexible scientific software ecosystem. This poster highlights work in four focus areas.

Use Cases: Three important BER use cases drive our work: climate impacts on the upper Colorado river system; hydrology and soil carbon dynamics of the Arctic tundra; and hydrologic, land surface, and atmospheric process coupling over the contiguous U.S. Recent use-case advances include adoption of more powerful source code management tools, expanded automated testing, and improvements in flexible multiphysics frameworks and interoperability of components that enable application scientists to focus on their areas of expertise while easily employing cutting-edge external software. See three IDEAS use-case posters led by C. Steefel, S. Painter, and L. Condon.

xSDK: A central activity is development of an Extreme-scale Scientific Software Development Kit (xSDK) — a collection of related and complementary software elements that provide the building blocks, tools, models, processes, and related artifacts for rapid and efficient development of high-quality applications. The second release of the xSDK in February 2017 included four numerical libraries (hypre , PETSc , SuperLU , and Trilinos) and two domain packages (the Alquimia geochemistry interface and the PFLOTTRAN subsurface application). Draft xSDK community package policies help to address challenges in interoperability and sustainability of software developed by diverse groups.

HowTo: To help improve developer productivity and software sustainability while ensuring continued scientific success, we are creating methodologies for *Productivity and Sustainability Improvement Plans (PSIPs)*. A PSIP is a tool for helping a software team to increase software quality while decreasing the effort, time, and cost to develop, deploy, maintain, and extend software over its intended lifetime. The PSIP workflow is intended to be lightweight and fit in with a project's standard planning and development process.

Outreach: The final piece of IDEAS is outreach and collaboration with the broader computational science and engineering (CSE) community. In spring 2017 we will launch a web-based portal as the hub of a community of interest/practice in software engineering for high-performance CSE.

Poster #216

Intermediate-scale Simulations of Thermal Hydrology of Polygonal Tundra

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Current environmental system simulation software tools often lack the flexibility to efficiently implement the thoughtful approximations that are critical to effective simulations of environmental systems. The Interoperable Design of Extreme-scale Application Software (IDEAS) project is addressing this barrier to productivity using integrated surface/subsurface thermal hydrology of thawing polygonal tundra as a use case. Simulating the soil thermal hydrology system in degrading permafrost regions is challenging because of strong coupling among thermal and hydrologic processes, the important role of organized microtopography in controlling water flows, strong coupling between the surface and subsurface, and the potential for topographic changes as ground ice melts. To address those challenges, we have implemented an intermediate-scale model using the ATS software (Painter et al. 2016). The computational strategy uses individual ice-wedge polygons as the horizontal discretization of the landscape. Associated with each ice-wedge polygon is a one-dimensional column comprising subsurface, a surface water reservoir, snow pack, and a surface energy balance. Those columns are simulated independently, then coupled indirectly through an overland flow system. Effects of neglected microtopography are included through subgrid parameterizations informed by fine-scale simulations. Results using this mixed-dimensional model structure compare well with fully three-dimensional simulations, but with significantly smaller computational burden. Projections of a 468-polygon region of the Barrow Environmental Observatory to year 2100 combine fine- and intermediate-scale simulations, and thus demonstrate part of the Next Generation Ecosystem Experiments-Arctic (NGEE-Arctic) scaling strategy. Inundation fractions extracted from those intermediate-scale simulations provide the additional link to climate-scale simulations. Simulations that include thaw-induced subsidence become tractable in our intermediate-scale model because the subsurface thermal hydrology and deformation processes are represented on independent one-dimensional columns. In addition, the mixed-dimensional spatial structure has broader applicability in watershed modeling. Managing the multiple meshes and multiple process representations in these intuitively appealing mixed-dimensional simulations is a significant software challenge. As part of the IDEAS project's broader goal of enabling a "virtual ecosystem" of composable software components, this Use Case demonstrates how a configurable model coupling system (Coon et al. 2016) can enable this class of multiscale, multiphysics models.

Poster #217

Advancing Integrated Hydrologic Modeling at the Continental Scale

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The first high-resolution integrated hydrologic model the continental US was developed for Use Case 3 of the Interoperable Design of Extreme-scale Application Software (IDEAS) project. This model covers 6.3 million km² at 1 km² spatial resolution, and incorporates dynamic interactions from the groundwater to the land surface using ParFlow-CLM. We employ this platform to simulate transient behavior based on historical meteorological forcings for several scenarios. Predevelopment simulations were used to evaluate the partitioning between evaporation and transpiration. Results demonstrate a novel connection between lateral groundwater flow and terrestrial water budgets. This work reconciles systematic differences between global observations and global land surface models. Additionally, predevelopment model outputs demonstrate that groundwater surface water exchanges systematically bias Budyko relationships between runoff and evapotranspiration in predictable ways. Building from the predevelopment scenario, we incorporate groundwater depletions that have occurred over the last century. Comparisons between depleted and predevelopment groundwater configurations demonstrate how large scale storage losses have fundamentally altered system dynamics. Next this anthropogenic signal will be compared to systematic warming in additional scenarios that reflect several levels of projected warming.

We are also working to expand the domain from coast-to-coast and increase the spatial resolution to 250 m². Lack of consistent subsurface data is one of the primary limitations of continental scale simulations. To facilitate this expansion, we developed the first US aquifer map including information on aquifer thicknesses and spatial distribution of alluvial aquifer systems and consolidated aquifers. Using this map, we have tested subsurface parameterizations and sensitivities in the high plains and central valley.

Through the collaboration with IDEAS, Use Case 3 has also explored improving the productivity of developers and scientists who work with ParFlow. In particular, ParFlow developers have updated several tools and practices based on best practice methodologies promoted through IDEAS and demonstrated in the Extreme-scale Scientific Software Development Kit (xSDK) exemplar package, Alquimia. These updates include, moving source code management to a public Git repository on the GitHub site, and leveraging tools there for issue tracking and continuous integration (e.g., Travis CI). In addition, a Software Productivity and Sustainability Plan was developed for ParFlow, which describes the development team's approach to software engineering methodologies that ensure a sustainable high-quality capability for the community. Finally, the team is exploring the componentization and interface design of its Land Model in order to release it to the community as a domain component in the xSDK.

IDEAS Use Case I: Improved process representation in watershed models across scales through software interoperability and productivity

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The need to understand and predict climate impacts and feedbacks on terrestrial ecosystems is driving an increased interest in models that represent and couple all relevant processes. But even as field and laboratory campaigns rise to the challenge of collecting diverse and heterogeneous datasets that can inform and constrain these models, questions remain about process representation and implementation. In this presentation, we summarize three activities we have performed to address different aspects of these questions in support of modeling efforts of Berkeley Lab's Watershed Function Scientific Focus Area at the East River watershed, Colorado. In particular, we (1) pursue code interoperability as an efficient means to add existing capabilities to codes that lack them (2) explore variable mesh resolution and refinement approaches to improve model accuracy in regions of interest, and (3) use model intercomparison to benchmark capabilities and build confidence in model results.

Code Interoperability. As our models become more elaborate and move toward multiscale representations, we need the ability to combine different computational processes and algorithms in a sensible and interoperable fashion. For example, we use Alquimia, an interoperable interface designed to provide biogeochemical processes to flow/transport models, to add biogeochemical capabilities to surface-subsurface codes ATS/Amanzi and Parflow. Current work focuses on the use of the new capabilities in the simulation biogeochemical transformations along a hillslope of the East River watershed.

Adaptive Mesh Refinement (AMR). AMR is a numerical technique for adjusting the resolution of computational grids near important features to enable more accurate calculations locally, and to reduce the computational burden of large domains. We have developed a surface-subsurface solver based on the kinematic wave and Richards equations using an AMR formulation. This approach may be particularly useful in accurately capturing water fluxes that develop in localized areas of the simulation domain.

Benchmarking. The community is increasingly turning to model intercomparison studies where multiple codes solve the same problem to expose and understand differences in results. While recent model intercomparisons in integrated hydrology have utilized simple geometries and small domains, we take a step further by tackling the complex and highly characterized topography associated with a meandering reach of the East River. Specifically, we compare three integrated hydrology codes ParFlow, Amanzi/ATS and the AMR-based code described above, which solve variably saturated subsurface flow using Richards equation coupled to surface water flow.

Subsurface Biogeochemical Research

University Awards

Poster #183

A Vegetative Facies-Based Multiscale Approach to Modeling Nutrient Transport

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The impact of submerged vegetation on nutrients and contaminants distribution in the Columbia Plateau region has been generally overlooked in recent multiscale modeling efforts. Yet, vegetation is the regulatory layer between many hydrological and ecological functions and plays a pivotal role in fluvial systems. One common challenge in modeling transport in vegetated rivers is the lack of predictive models linking vegetation type and topology with effective transport properties of the vegetative layer itself and its dynamic linkages to its surroundings (i.e. groundwater and surface waters). Specifically, existing models provide only limited understanding of the mechanistic connection between vegetation topology and its function. We address this challenge by modeling the vegetated layer as a porous medium. Such an underlying hypothesis allows us (i) to establish a mechanistic relationship between vegetation structure (e.g. LAI, height, density) and function (permeability, effective dispersion and reaction rates of the canopy layer), and (ii) to construct a framework, and corresponding mathematical machinery, to model the impact of vegetation on nutrient cycling.

Poster #162

A Last Line of Defense: Understanding Unique Coupled Abiotic/Biotic Processes at Upwelling Groundwater Interfaces

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Groundwater seeping from sediments into lakes, wetlands, and rivers generates approximately 70% of total surface water flow in the USA. However, groundwater can carry excess nutrients and other contaminants, and therefore threaten surface water quality. Fortunately, the shallow interface sediments that line surface water bodies can host beneficial bacteria that naturally remove contaminants from groundwater as it strains through pores on the way to the surface. When water that is low in dissolved oxygen reaches the oxygenated surface water, metal (typically Fe, Mn) oxides may be deposited in layers 10's of cm thick. These soupy deposits of iron (red) and manganese (black) metals are often observed around wetlands at groundwater seeps, or can coat solid grains in faster flowing systems such as the East River, CO. These deposits of metal oxides, which are also observed in abundance within mine-impacted watersheds, act as "contaminant sponges" that sorb toxic compounds. These toxins include arsenic and uranium, which threaten animal and human health. However, dissolved oxygen levels in surface and shallow groundwaters are highly dynamic, and if oxygen with shallow interface sediments is decreased, metal oxides may dissolve and their contaminants may be released as a toxic pulse.

The hydraulic pressures that affect oxygen exchange, and in turn, drive metal-oxide deposition and dissolution are complicated and currently not well defined. Further, there is emerging evidence that the metal-oxide deposits may act as strong conductors of heat and electricity, which likely affects sediment reaction rates including carbon cycling and the contaminant sequestration. We plan to extensively study metal oxides in the laboratory and within a mine-impacted watershed in Colorado to: (1) better understand how dissolved carbon and contaminants pass from groundwater to surface water, and (2) capitalize on the ability of natural systems to adsorb and sequester contaminants. This study will result in predictive, processes-based understanding of the paired stream and groundwater conditions that lead to metal-oxide deposition so our water resources can be better managed and used.

Poster #193

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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Historical and ongoing releases of mercury (Hg) have resulted in a legacy of Hg contamination in streambed sediment, stream banks, 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, stream banks, 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 the Lower EFPC suggest that additional dissolved Hg from either the hyporheic zone, riparian wetlands, or groundwater discharge may variably contribute as much as 16-80% of downstream dissolved Hg loads during base flow conditions. Thus, one of the over-arching goals 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 and drive observations of watershed-scale mercury fluxes. To achieve this goal, we are coupling the Hg isotopic composition of dissolved Hg in stream water and in critical subsurface ecosystem compartments (i.e., hyporheic zone, riparian wetlands, 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.

During the first six months of this project we have: (1) initiated monthly base flow surface water sampling to characterize changes in the concentration and isotopic composition of dissolved Hg in each of four gauged reaches of the EFPC; (2) installed infrastructure (semi-permanent piezometers) for sampling hyporheic pore water; and (3) collected the first seasonal sampling of hyporheic pore water and riparian groundwater from five locations along the flow path of the Lower EFPC. Here, we present dissolved Hg concentration and Hg isotopic composition of all surface water, hyporheic pore water, and riparian groundwater samples analyzed to date, and begin to make mass balance assessments regarding legacy inputs of dissolved Hg to the stream water of EFPC.

Poster #203

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, such as uranium, 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.

An important control on carbon cycling within soils and sediments is constraints on microbial metabolisms induced by the respiratory pathway, and specifically the electron acceptor in respiration, which further serves to control metal fate and transport. Within floodplain soils and sediments, variations in hydrologic state (water saturation) coupled with structured porous media lead to extensive heterogeneity in redox environments and thus metabolic trajectories controlling organic carbon oxidation.

Combining micro-scale laboratory experiments with field-scale observations, we find that oxygen diffusion limitations lead to heterogeneous redox profiles, shifting microbial metabolism to less efficient anaerobic SOC oxidation pathways. In both saturated and unsaturated systems, microsensor measurements in combination with gas flux measurements showed that particle size exerts a strong control on the extent of the anaerobic volume, thereby causing an overall decrease in OM oxidation rates. In model soils and sediments, we determined the distribution of operative microbial metabolisms and their cumulative impact on SOM transformations and overall oxidation rates within anaerobic microsites. Metabolic profiling showed that texture-induced anaerobic microsites reduced carbon oxidation rates by an order of magnitude relative to aerobic rates, with Fe reduction contributing more than 75% of the overall metabolism. Density separations in combination with C 1s NEXAFS spectroscopy and high-resolution FT-ICR-MS showed that texture-induced anaerobic microsites resulted in the preferential preservation of reduced (electron-rich) organic carbon compounds (both dissolved and particulate), a result corroborated by field measurements across multiple sites. Near-edge X-ray absorption spectroscopy similarly indicates a loss of oxidized functional groups within the anaerobic domain.

Collectively, our results suggest that anaerobic zones have prominent controls on organic carbon oxidation in both saturated and unsaturated soil/sediment, thermodynamically stranding reduced carbon compounds. Removing anaerobic metabolic constraints upon a shift in oxygenation will stimulate microbial oxidation of thermodynamically protected carbon.

Poster #218

Sensitivity of Transpiration to Subsurface Properties

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The amount of moisture transpired by vegetation is critically tied to the moisture supply accessible to the root zone. In a Mediterranean climate, integrated evapotranspiration (ET) is typically greater in the dry summer when there is an uninterrupted period of high insolation. We present a 1D model to explore the factors that may sustain ET. The model includes a stochastic parameterization of hydraulic conductivity, root water uptake efficiency and hydraulic redistribution by plant roots. Model experiments vary the precipitation, the seasonality of ET demand, and rooting profiles and rooting depths of the vegetation. The results show that the amount of subsurface moisture remaining at the end of the wet winter is determined by the competition between abundant precipitation input, fast infiltration and winter ET demand. In a Mediterranean climate, weathered bedrock provides a not-insignificant reservoir that may sustain ET of deep-rooted (>8m) trees through the dry season. A small negative feedback exists in the root zone, where the depletion of moisture by ET decreases hydraulic conductivity and enhances the retention of moisture. Hence, hydraulic conductivity is impactful in a dry season or a dry year when hydraulic conductivity is reduced, or at a location with less permeable lithology.

Poster #184

Transport and Transformation of Particulate Organic Matter in Permeable Riverbed Sediments

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Rivers and other inland water systems are key sites of biogeochemical transformation and storage; they are also distinct ecosystems, geomorphological agents and conduits for material transport across continents to the oceans. Biogeochemical activity in rivers is often conceptualized as occurring predominantly in the water column. However, by far the largest amount of biogeochemical activity takes place within the riverbed, either at or just below the surface. This occurs because the concentration of organic matter (OM) and associated microorganisms is several orders of magnitude higher than the concentration in the water column. Such dynamics have fundamental implications for CO₂ and/or CH₄ production and efflux as well as retention and/or release and transport flux of other nutrients (e.g. N, P) associated with POM decomposition.

Our project is initiating a program of research to examine riverbed Particulate Organic Matter (POM) transport and biogeochemistry in Columbia River (CR) sediments, leveraging knowledge developed as part of the PNNL Science Focus Area (SFA). In particular, we are characterizing POM transport and transformation in simulated, near-shore CR sediments through a series of column experiments. This research is designed to lay the foundation for future experiments and in situ observations characterizing biogeochemical processes associated with POM accumulation and transformation in actual permeable riverbed sediments. The primary goals of this limited set of experiments are to (1) determine the physiochemical processes controlling the POM transport and accumulation within simulated riverine sediments, (2) quantify microbial respiratory metabolism and POM mineralization driven by this accumulation. In addition, we will develop a 1-dimensional transport-reaction model of POM accumulation and metabolism that can be utilized in future experimental studies and could eventually be incorporated into ongoing simulations of hydrological transport and biogeochemical activity in the Hanford 300 Area SIZ.

Current research efforts are focused on quantifying the short-term (< 0.5 day) accumulation of POM in simulated, permeable riverbed sediment. We have examined the transport and accumulation of fresh algal POM in column reactors packed with Hanford sand and fine-grained silt and clay. Parallel experiments are being conducted with latex spheres with an equivalent diameter to the POM. By examining the comparative behavior of the POM and non-living latex spheres will have determined that surface properties of particles and sediment play a critical role in POM transport behavior. The next phase of our research will investigate longer-term (2-4 week) decomposition dynamics of POM in permeable sediments.

Poster #163

A Multiscale Approach to Modeling Carbon Cycling Within a High Elevation Watershed

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The rates of soil carbon accumulation, transformation and release to the atmosphere and surface waters remain a key uncertainty in global-scale models. Within the soil environment, residual plant material is transformed into a continuum of organic products of variable accessibility and reactivity. At the watershed scale, averaging over complex soil reaction networks may obscure critical processes; whereas individual soil profiles provide a limited view of the ensemble of pathways that ultimately determines carbon fluxes. To address how collections of spatially and temporally linked reaction networks are manifest at larger scales and the consequences of scale for process-based models, we are studying C fluxes at molecular-level all the way to the watershed-scale within the LBNL SFA East River, CO watershed study site.

To date, we have characterized landscape-scale carbon fluxes within the upper catchment using concentration-discharge relationships and through distributed soil sampling and flux measurements. To understand the biogeochemical and hydrologic dynamics driving these fluxes, we developed two microcatchment study sites at different elevations and life zones (2950 and 3500 m; upper montane and upper subalpine) where we have depth-resolved soil moisture and temperature sensors, soil gas wells and lysimeters paired with measurements of soil surface CO₂ fluxes. Newly developed spectroscopic methods for characterizing molecular-level soil carbon speciation are coupled to field measurements. The depth-resolved CO₂ concentrations suggest that the depth of maximum respiration rates increases throughout the growing season, likely reflecting seasonal drying and the downward movement of optimal soil moisture conditions. An inverse-model of respiration rates suggests two local maxima at shallow (~25 cm) and deep (100-150 cm) depths. This is supported by differences between the observed pCO₂ and model simulations of the microbial dynamics constrained by incubation experiments, indicating that root respiration is vertically offset from the maximum microbial respiration. Collectively, our combined modeling and data collection suggest that vertical movement of water and seasonal shifts in soil moisture distribution are a critical control on subsurface respiration rates that will need to be accounted for in large-scale models.

Poster #164

Experimental and Modeling Investigation of the Impact of Atmospherically Deposited Phosphorus on Terrestrial Soil Nutrient and Carbon Cycling, and Ecosystem Productivity

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An accepted paradigm of terrestrial ecosystems in temperate climates is that nitrogen (N) rather than phosphorus (P) is the dominant limiting nutrient to plant growth. Recent studies, however, suggest that the anthropogenic release of large quantities of oxides of N into the atmosphere through fossil fuel combustion has greatly enhanced N inputs to ecosystems, such that the bioavailability of P rather than N may now control terrestrial productivity. Furthermore, even in relative pristine environments that have low N inputs from the atmosphere but where the soil is derived from low P-bearing geological substrates, P may also regulate ecosystem productivity and the removal of the primary greenhouse gas carbon dioxide from the atmosphere. In this exploratory project, we are using a combination of spectroscopic methods, stable isotopes, and selective chemical extractions to determine labile or recalcitrant P species, and to evaluate sources and changes in P speciation with atmospheric deposition to soil. We are examining initial samples collected in Sept.-Oct. 2016 from two montane sites: one along a well-established altitudinal transect in the Southern Sierra Critical Zone Observatory (SSCZO), and one in the East River Watershed in Upper Colorado River Basin (in collaboration with Lawrence Berkeley National Laboratory (LBNL)). Samples were collected using passive air sampling (static pans) placed at two different elevations at each location. Particulates were washed from the pans, filtered sequentially through 10 and 0.2 micrometer PTFE Teflon filters, and air-dried. X-ray absorption spectroscopy (XAS) at the P K-edge of bulk material on filters showed differences among the two locations and two elevations in both the energy position of the maximum absorbance and in post-maximum edge features. These spectra, in comparison with solid phase reference compounds and phosphate sorbed on mineral surfaces, indicate mixtures of several P species in the dust samples. Further characterization by electron microscopy, solid-state ³¹P NMR, and stable isotopes ($\delta^{18}\text{O}$ in PO_4) is ongoing, as well as chemical analyses and selective extraction. Snow sampling will occur in spring 2017 followed by summer sampling in order to compare differences among particulate material deposited at different times of the year. These studies will help establish whether the chemical forms of P from atmospheric particle deposition have significant reactivity for incorporation into soil biogeochemical cycles, and thus may have a potentially large and disproportionate impact on net ecosystem productivity in P-limited terrestrial ecosystems.

Poster #208

Imaging Radionuclide Transport in Porous Media

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This project is a part of Department of Energy, Experimental Program to Stimulate Competitive Research (EPSCoR) Implementation Grant “*Radionuclide Waste Disposal: Development of Multi-scale Experimental and Modeling Capabilities*”. It includes a combination of lab and field experiments over scales ranging from micrometers to decimeters. A variety of imaging modalities are utilized to image flow and transport processes through pore, column, and lysimeter scales.

1D scans of gamma-ray emitting contaminants have been conducted on lysimeters from the RadFLEX facility at the Savannah River Nationals Laboratory (SRNL). Following weathering of radionuclide contained within a cementitious wastefrom or incorporated into soil for three to four years, the spatial distribution of the radionuclide was quantified with 2.5 mm resolution. These scans showed downward mobility of cobalt-60 and barium-133 when the radionuclides were incorporated directly into the SRNL soil. When radionuclides were incorporated into the cementitious wastefrom positioned in the SRNL soil, cesium-137 exhibited both upward and downward dispersion while the other radionuclides showed no movement. Europium-152 was the only radionuclide of those studied that showed no movement from the original placement within the lysimeter.

Preclinical x-ray computed tomography (CT) technique was used to image macropores and preferential flow paths in the lab columns. Single photon emission computed tomography (SPECT) method, in combination with CT, allowed us to map 3D in-situ contaminant concentration distribution and relate anomalies in transport with the structural features in the porous media. These both methods were used to image the movement, absorption and retention of radionuclides in artificial (such as silica gel, glass beads, filter papers) and natural (SRS soil) materials.

Poster #209

Radionuclide Waste Disposal: Development of Multi-scale Experimental and Modeling Capabilities

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This abstract provides a general overview of a DOE Experimental Program to Stimulate Competitive Research (EPSCoR) Implementation grant in South Carolina with supporting funding coming from the BES Heavy Element Chemistry program and the BER Subsurface Biogeochemical Research Program. The objective of this project is to quantitatively describe the influence of coupled physical, chemical, and biological reactions on the migration of radionuclides through porous media. Particular emphasis is placed on determining processes which limit the rates of radionuclide migration including:

1. Impacts of fluid flow, particularly preferential flow, which induce chemical gradients and control the availability of reagents which may influence the mobility of radionuclides.
2. Identification of rate limiting steps of chemical reactions which cause changes in radionuclide mobility as well as the extent of reaction reversibility
3. Characterization of the time and length scales over which non-equilibrium states are maintained based on a competition between chemical reaction rates and physical processes (i.e. flow).

To meet these objectives, we will develop a series of novel, multidimensional tools capable of real time monitoring radionuclide mobility in space and time. This effort will entail development of 2D sensors to monitor chemical states and distribution (i.e. pH, O₂(aq) concentrations, radionuclide concentrations) in 2D microfluidic cells and macroscale tanks as well as CT and SPECT medical imaging techniques to monitor flow, pore structure, and radionuclide distribution in 4D.

Highlights from several ongoing experimental and modeling studies will be discussed including:

1. Examination of uranyl phosphate dissolution by plant exudates using batch flow through reactors, 2D microfluidic systems, and soil column testing.
2. Development of novel 2D and 3D measurement techniques including x-ray CT and Single Photon Computed Tomography (SPECT) examining Tc-99m transport through porous media. We have evaluated the spatial and temporal resolution limitations of these techniques in an idealized system (i.e. Tc-99m transport through a column packed with glass beads of varying sizes) and also monitored redox driven retention of Tc-99m through soil columns with heterogeneous reducing zones.
3. Quantification of sorption hysteresis and rate limiting steps involved with Cs ion exchange on a sandy loam soil and iodine transformations to organo-iodine species in a wetland sediment. Both studies indicate there is a low concentration but highly reactive component of the soil which controls Cs and I behavior at environmentally relevant concentrations.
4. Field based lysimeter studies of Tc-99 and Np-237 which indicate Tc-99 and Np-237 mobility are highly controlled by oxidation of initially Tc(IV) and Np(IV) sources. The rate and extent of source term oxidation was examined through measurements of Np and Tc in the lysimeter effluents during field deployment as well as leaching, batch sorption, x-ray absorption spectroscopy, and electron microscopy techniques after the lysimeters were retrieved from the field.

Poster #210

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

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Background: a) ¹²⁹I is among the top three risk drivers at DOE Low Level Waste or High Level Waste disposal sites, such as Savannah River Site (SRS). Radioiodine's risk stems largely from its perceived high environmental mobility, large inventory (high fission yield), high toxicity (it is a thyroid seeker), and long half-life (16M years). ¹²⁹I exists as multiple species (usually iodide, iodate, and organo-iodine). **b)** The human and environmental risks associated with Pu disposal, remediation, and nuclear accidents scenarios stems mainly from the very long half-lives of several of its isotopes. The SRS, holding one third of the nation's Pu inventory, has a long-term stewardship commitment to investigation of Pu behavior in the environment.

Methods: a) Six different genera of Mn(II)-oxidizing bacteria were isolated from SRS soils, and examined for the ability to oxidize iodide directly through enzymatic catalysis, or indirectly through formation of reactive oxygen species (ROS) and/or biogenic manganese oxides. **b)** Humic substances (HAs) from different types of soils in various global regions, were re-suspended with groundwater at a far-field Pu concentration (10^{-14} M) to examine the influence of natural organic matter (NOM) on Pu partitioning during soil erosion events.

Results: Both extracellular enzymes and ROS play a role in microbial Mn(II)-oxidation. Iodide oxidation was not observed in cultures of the most active Mn-oxidizing bacteria. While substantial amounts of Mn(III/IV) oxides were only generated in cultures \geq pH 6, iodide oxidation was only observed in the presence of Mn(III/IV) oxides when the pH was \leq 5. Iodide oxidation was promoted to a greater extent by synthetic Mn(IV)O₂ than biogenic Mn(III/IV) oxides under these low pH conditions (\leq pH 5). Thus, the influence of biogenic manganese oxides on iodide oxidation and immobilization is primarily limited to low pH environments.

b) Under acidic condition (pH~5.5 as the global averaged soil pH), $29 \pm 24\%$ of organic matter was released from the HAs, carrying $76 \pm 13\%$ of total added Pu into mobile colloidal phase. Both Pu activity concentration and partitioning coefficients (LogKd) were strongly and positively correlated with nitrogen contents in both particulate and colloidal fractions. Results from solid state ¹³C NMR suggest carboxylate functionalities contribute to the particulate-immobilization and colloidal-remobilization of Pu during HA37 groundwater resuspension. Carboxyl- and nitrogen-containing organic moieties in the bulk NOM pool served as the predominant Pu carrier, which is relevant to potential Pu mobility in natural soils during surface runoff events.

Poster #165

Mechanistic and Predictive Understanding of Needle Litter Decay in Semi-Arid Mountain Ecosystems Experiencing Unprecedented Vegetation Mortality

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The Rocky Mountains of North America are experiencing a prolonged period of ecological stress resulting from coupled human and natural disturbances including logging, wildfire mitigation and incidence, climate change, and large scale insect infestation. The latter have decimated tree populations across millions of acres of forest in the region with repercussions for biogeochemical processes that can influence water resources, ecosystem function, and human well-being. The current exploratory project focuses on the decay of needle litter as a function of beetle impacted vs. unimpacted spruce (*Picea pungens*) in complement to lodgepole pine given their relevance to this form of large-scale disruption in the region. Needles were harvested from geographically similar sites and then deployed within the East River watershed at different elevations in fall 2016 to understand the effect of temperature, moisture, accelerated snowmelt and differing needle chemistry on decay processes and carbon and nitrogen export into the atmosphere (i.e. CO₂ and N₂O) and hydrosphere (i.e. nitrate, ammonia, DOC). In isolating the needles from the hydrodynamic and biogeochemical variables of the tree system, our goal is to better understand the relative biogeochemical contributions of needle decay versus rhizospheric processes in distressed ecosystems. Ultimately this necessitates contrasting these processes with those under trees, where we propose to investigate plots of spruce trees in a nearby watershed that contains both beetle-killed and non-impacted spruce. In addition to enabling an understanding of these intertwined processes on biogeochemical cycling, this will enable us to query how localized treescale hydrologic and biogeochemical responses scale to watershed processes and the potential compensatory effects of healthy surrounding trees. Collectively, our research has implications for forest recovery and nitrogen export in this nitrogen-limited montane ecosystem and could aid in the prediction of and preparation for biogeochemical shifts that could impact water quality or greenhouse gas release.

Poster #194

From Atomic Scale to Macroscopic Modeling: A Multi-Scale Framework for Mercury Biogeochemistry

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Predicting the environmental fate and transport of mercury (Hg) in terrestrial surface and subsurface systems requires a thorough and accurate description of its speciation. Continuum-scale geochemical modeling typically employs experimentally determined thermodynamic binding constants (e.g., “log K ”) to model the transport and transformations of metals in the environment. However, the application of this method to Hg biogeochemistry is often limited due to the lack of reliable thermodynamic data. For example, the experimentally measured log K values for Hg complexation with highly variable natural organic matter (NOM) span a considerable range of >35 log units. Furthermore, even within a single well-defined system, such as Hg(Cys)₂, literature values vary by >20 log units. To this end, we have generated an aqueous speciation database for Hg complexes by combining high-quality experimental data adherent to IUPAC standards with theoretical data calculated with density functional theory (DFT). Currently, the database includes over 500 experimental records for 152 inorganic and organic compounds, and continues to expand. We extend our previous work in applying DFT to predict the thermodynamic constants of Hg complexes uncertain or otherwise not available in the literature and integrate the results of 86 reactions calculated using 12 different DFT methods into the database. Further refinement of this database will provide a data resource for predicting speciation of Hg and other molecular species as well, and will therefore enable the application of the continuum-scale modeling to study Hg biogeochemistry. Future studies will focus on calibrating and improving the accuracy of the current DFT prediction model, and on linking the atomistic models to the macroscopic continuum-scale modeling framework to predict the transport and transformation of Hg in the environment.

Poster #166

PAF: A Cloud Based Framework for Site Monitoring

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Water resource management, agriculture and contaminated site remediation all require a timely understanding of subsurface processes to support operational efforts. This understanding requires the autonomous application of multi scale, multi domain models which are parameterized by heterogeneous multi scale data (geophysical, geochemical, hydrological and remote sensing) and the distillation of data and model outcomes into actionable information.

Under DOE SBIR award DE-SC0009732 Subsurface Insights in collaboration with LBNL scientists has developed the modular cloud based software framework PAF (Predictive Assimilation Framework) for providing this actionable information. PAF was designed from the ground up to provide a vertically integrated platform for all tasks ranging from heterogeneous data ingestion, qa/qc, data processing, parameter estimation, modeling, result sharing and information generation.

To achieve this PAF extensively leverages open source codes and capabilities for data ingestion, processing and modeling, including Landlab and PFLOTRAN (modeling), E4D (electrical geophysical data processing), ODM2 (Data storage), R (statistics), QGIS (data visualization and processing) and TikiWiki (knowledgebase).

Data is stored in a variety of ways including standard relational database (Mysql/PostGIS) and NoSQL solutions such as HDF5 data for storage of model results and Distributed Temperature Data. PAF uses configurable python workflows for back end tasks (such as data ingestion/harvesting and processing) which allows for rapid extension of capabilities as well as the use of the built in capabilities provided by Python for data processing and image manipulation. Within PAF, data and capabilities are exposed through APIs (either native to the open source component or developed in house) allowing for easy integration between components. PAF uses Zend Framework 2, a PHP 7 web application framework in the backend. Users interact with PAF through standard browsers and IOS and Android Apps. PAF is being developed and validated with data from different sites including the LBNL East River site. Specifically, we are currently extending PAF to include coupled surface/subsurface processes occurring between the bedrock and the soil/atmosphere interface. PAF: a cloud based framework for site monitoring

Poster #167

Characterization of Groundwater Flow and Associated Geochemical Fluxes in Mineralized and Unmineralized Bedrock in the Upper East River and Adjacent Watersheds, Colorado

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This project is just beginning in 2017. We intend to combine multi-scale interdisciplinary strategies for improving the state of knowledge regarding the influence of deep-circulating groundwater on stream flows and stream-water chemistry in mountain watersheds. Like many rivers with alpine headwaters, the East River watershed contains several zones of exposed mineralized and hydrothermally altered bedrock. Surface and groundwater draining these mineralized zones commonly contains high concentrations of metals and other solutes due to an abundance of metal sulfide minerals in the aquifers, and can contribute substantially to stream chemical loads. We will compare how the fluxes of metals and other solutes to the surface varies between mineralized and unmineralized areas within the upper East River watershed and adjacent areas near Crested Butte, Colorado. This work will complement the ongoing ecohydrologic Science Focus Area (SFA) project led by the Lawrence Berkeley National Laboratory (LBNL) that includes extensive sampling and analysis of near-surface materials and surface waters by: (1) collecting new data in mineralized areas to contrast with the unmineralized East River study area, and (2) focusing on the contribution of deep-circulating groundwater and its geochemical composition to the shallow flow system. The aim of the proposed work is to develop a conceptual model of the deep bedrock hydrogeochemical system in both mineralized and unmineralized areas of the upper East River that could provide the foundation for incorporating the deeper subsurface into the numerical reactive transport model being developed for the watershed by LBNL. Our results will enrich the ongoing LBNL studies by providing a more robust understanding of the hydrogeologic system and help forecast the effects of perturbations such as climate change. We will combine new borehole installations with geologic, geophysical, geochemical, and hydrologic characterization of the deeper subsurface that extends 10s to 100s of meters below ground to better understand and quantify fluxes of water, metals, and other solutes from deeper to shallower environments.

Poster #168

Hyporheic Mixing as a Strong Controller of Riverbed Biogeochemistry in Low-Order River Networks

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Hyporheic mixing between river water and groundwater is hypothesized to exert a strong influence on riverbed biogeochemistry in low-order streams and rivers. Indeed, mixing zones near the sediment-water interface are thought to be hotspots of biogeochemical activity. In the semi-arid western US where river discharge is dominated by snow-melt, the seasonal expansion and contraction of the hyporheic zone likely exposes the riverbed to alternating oxic and anoxic conditions, with implications for reactions affecting metal mobilization and carbon processing. A greater understanding of these interdependent processes is critical for predicting the export of nutrients from upland watersheds, tracking metal mobilization in contaminated regions, and modeling the future behavior of river biogeochemistry in a changing climate.

Working around a representative meander feature of the East River (Crested Butte, CO), we used a series of vertically resolved temperature and redox probes to track the extent of hyporheic mixing, and the impact of mixing on riverbed biogeochemical processes. Pore water temperature data collected between August, 2016 and February, 2017 revealed a greater river water influence in the point bar location and a greater groundwater influence at the meander apex and cut bank locations. Groundwater upwelling increased at the cut bank location throughout the summer and fall. In winter, the onset of riverbed freezing occurred later at the groundwater-influenced locations, thus sustaining conditions necessary for microbial activity throughout more of the year. Further evidence for strong groundwater influence in shallow regions of the riverbed was obtained through depth-resolved pore water sampling at discrete time points. Characteristic of anaerobic microbial metabolism, aqueous metal (iron, manganese) concentrations increased with depth, while sulfate decreased over the same vertical profile. Furthermore, evidence of aerobic respiration (through oxygen consumption measurements) was mostly confined to the upper 20-cm of sediments. Ongoing 16S rRNA gene and metagenomic analyses will provide greater insight into the distribution of microbial metabolisms through the sampled zones.

In late-Spring 2017, complementary pore water samples will be collected during high river discharge to measure the effects of strong river water down-welling on riverbed biogeochemistry. Combined biogeochemical datasets will be used to develop coupled reactive transport and microbial population models in the riverbed. These models will be used to quantify reactive solute exchange across the riverbed and microbial population dynamics under various seasonal signals. In particular, we will explore potential impacts of future changes in precipitation, snowmelt, and river discharge on hyporheic mixing and associated biogeochemical processes.

Poster #195

Biogeochemical Release and Reactions of Iron-Bound Organic Carbon During the Redox Processes

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Iron (Fe)-bound organic carbon (OC) contributes an important component in the global cycles of OC. In this project, we have systematically studied the biogeochemical reactions of Fe-bound OC during the redox processes.

We have investigated the release and transformation of synthesized Fe-OC complexes during the abiotic and biotic reduction. During the abiotic reduction, hematite-bound OC was released more rapidly compared to the reduction of Fe, and aliphatic OC was more resistant to the reductive release than other components of OC. In the microbial reduction, reduction of ferrihydrite (Fh) and reductive release of Fh-bound OC were governed by the C/Fe ratio, with higher C/Fe ratio enhancing the Fe reduction and release of Fe-bound OC. In addition, we synthesized Fh coprecipitated with model OC, including glucose (GL), glucosamine (GN), tyrosine (TN), benzoquinone (BQ), amylose (AM), and alginate (AL). During the 25-d reduction by *Shewanella putrefaciens* CN32, the reductive release of OC followed the order Fh-BQ > Fh-GN > Fh-TN > Fh-GL > Fh-AL ≈ Fh-AM. OC regulated the reduction of Fh through acting as an electron shuttle and affecting the bacterial activity. Our results showed that the Fe reduction and release of Fe-bound OC were governed by the mineral phase of Fe oxide, C/Fe ratio, and chemical composition of OC.

For natural forest soils, Fe-bound OC contributed about 38% of total OC in forest soils. The anaerobic release of OC was closely related to the microbial reduction of Fe. When soils were transferred to aerobic conditions, the mineralization of OC was substantially inhibited compared to soils without pre-reduction. The OC was sequestered potentially through the co-precipitation with Fh formed during the oxidation of Fe(II). Oxidation of Fe(II) by O₂ led to the generation of OH radicals, which dominated the abiotic oxidation of OC. These findings provide a novel insight into the role of redox reactions in the biogeochemical cycles of OC. We also have monitored the seasonal dynamics of CO₂ and CH₄ for tundra soils at Toolik site, and analyzed the microbial community in these soils through 16S rRNA analysis.

Through experimental studies on the synthesized complexes and natural soils, our results uncover the coupled dynamics of Fe reduction and OC transformation, i.e. the release of OC during anaerobic reduction and inhibited mineralization under aerobic conditions. For the next step, we plan to study the long-term respiration of Fe-bound OC under different temperatures and transformation of different functional groups during the redox processes.

Poster #196

Investigating Greenhouse Gas Fluxes in Tundra Soils *in situ* in the Field and Under Controlled Laboratory Conditions

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Arctic tundra soils contain significant amounts of organic carbon that can potentially release greenhouse gases such as methane (CH₄) and carbon dioxide (CO₂), particularly during freeze-thaw cycles. As the atmospheric lifetime and radiative forcing of each of these species differs, it is important to understand the mechanisms by which carbon release may preferentially be in favour of one species over the other.

We present 2 years of *in situ* observations of CH₄ and CO₂ soil concentrations in the Arctic tundra at Toolik Field Station in northern Alaska by diffusive gas wells. Field observations show a consistent production of CO₂ in all six gas wells, including throughout the arctic winter at soil temperatures below -15°C. Field observations showed both net oxidation of CH₄ and production of CO₂ in tundra soils within close proximity. A critical observation was that the production of CH₄ continued throughout the arctic winter, but oxidation of CH₄ ceased during the coldest period, suggesting different temperature sensitivities of the two processes leading to changes in net ecosystem CH₄ production.

To further investigate temperature sensitivities for tundra CO₂ and CH₄ dynamics, we conducted controlled laboratory incubations studies using flux chambers whereby temperatures were shifted incrementally between -10°C and 5°C. Initial results show cessation all oxidation and production of greenhouse gases (GHG) below -1°C, in contrast to field measurements that showed activity to continue under much colder temperatures. Net CH₄ fluxes altered with soil type and temperature, whereby O and A horizon soils showed net oxidation above 2°C when thawing, yet the net oxidation flux continued below 1°C during freezing. B horizon soil showed net CH₄ production above -1°C when thawing, yet this flux stopped at 1°C when freezing. These results show different temperature sensitivity of GHG production and oxidation in different soil horizons as well as differences between thawing and freezing processes.

Poster #169

Understanding Hydrobiogeochemical Drivers of Metal Export from Coal Creek, Colorado

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This project aims to develop predictive understanding of *key drivers of metal export at the watershed scale*. Metals association with dissolved organic carbon (DOC) is well documented at the laboratory scale. Preliminary data for Coal Creek, Colorado, have indicated similar connections – the concentration and discharge relationships of metals such as Cd and Zn mirror those of DOC demonstrating strong flushing (chemodynamic) behavior, in contrast to the chemostatic behavior of geogenic species that are the products of chemical weathering. In other words, in the high elevation Coal Creek watershed, most metal export occurs during the high flow - spring melt period (4.5% of the time), contributing disproportionately high fractions of 37% and 49% to the total annual water and DOC export, respectively. In this project we will 1) develop an integrated hydrobiogeochemical model at the watershed scale to systematically explore the connections among hydrological processes, soil carbon decomposition into DOC, and metal export; 2) apply the model to understand key drivers of metal export from Coal Creek.

In particular, we are developing a bioreactive module bio-RT to simulate processes including soil carbon stabilization, soil carbon decomposition into DOC, as well as complexation between DOC and metals. The module will be written in general framework and not for a particular watershed. All specifics of particular biogeochemical systems and watersheds will be communicated through input and output files. We will ultimately integrate bioRT into the IDEAS codes. Such a modeling tool is important not only for Coal Creek, CO, but also for other human-impacted watersheds including those in Appalachian Basin that extends thousands of miles. Human activities including historical mining and current natural gas production have threatened water resources that are important for tens of million people. Predicting capabilities are also essential in understanding the responses of these contaminated watersheds to changing climate.

DOE Scientific User Facilities

Poster #H1

The DOE Joint Genome Institute: A User Facility for Environmental & Energy Genomics

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The mission of the U.S. Department of Energy Joint Genome Institute (DOE JGI), a DOE Office of Science User Facility operated by Lawrence Berkeley National Laboratory, is to advance genomics in support of the DOE missions in bioenergy, carbon cycling and biogeochemistry. The Community Science Program (CSP) provides the scientific community access to high-throughput sequencing, computational analysis, DNA design and synthesis, and metabolomics for projects of relevance to DOE missions. In addition to the CSP, we have established collaborative programs with the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (PNNL) for molecular characterization and the National Energy Research Scientific Computing Center (NERSC) for computational capacity. We also partner with external groups through the Emerging Technologies Opportunity Program (ETOP) to develop cutting-edge technologies that can be translated to a high-throughput production environment for the larger scientific community. The DOE JGI has made significant contributions in environmental system science and continues to evolve as a state-of-the-art genomic science user facility.

www.jgi.doe.gov

Poster #H2

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

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Robust, predictive models of elemental cycling in terrestrial ecosystems and contaminant fate and transport in the subsurface require understanding and identification of key geochemical and biogeochemical 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 porescale simulation and PFLOTRAN, Amanzi and eSTOMP for continuum-scale simulation.

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

Poster #225

Characterizing Metallo-Organic Species Involved in Biological Metal Acquisition from Soils Using Advanced Mass Spectrometry

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Many elements are scarcely soluble in aqueous conditions found in soils unless complexed to strong binding organic ligands. To overcome this limitation, some plants and microbes produce chelators that solubilize micronutrient metals such as Fe, Ni, Cu, and Zn from mineral phases. These complexes are taken up by organisms via specific membrane receptors, thereby differentially impacting the bioavailability of these metals to the plant and microbial community. Although the importance of these chelation strategies for individual organisms has been well established, little is known about which pathways coexist in natural systems or how they interact and compete for metal binding. Identifying these metallo-organic species within environmental systems has remained a formidable analytical challenge due to the vast diversity of compounds and poorly defined metabolic processes in complex soil matrix. Fourier transform mass spectrometry (FTMS) offers the mass resolving power and accuracy required to resolve the unique isotopic signatures of many trace element containing compounds. In particular, the novel high magnetic field (21T) Fourier transform ion cyclotron resonance (FTICR) mass spectrometer at EMSL provides a unique combination of fast spectral acquisition rate, resolving power, accuracy and sensitivity needed to identify metal isotopologues on a liquid chromatography (LC) timescale. The same separation platform can also be combined with inductively coupled plasma mass spectrometry (ICPMS) to identify and quantify metal complexes. Herein, we employed recently developed LC-ICPMS-FTMS methods to characterize the speciation of water-soluble dissolved trace elements (e.g. Fe, Ni, Cu, and Zn) from soils. Samples were separated with reversed-phase (RP) LC and the eluent was analyzed by tandem quadrupole ICP-MS to detect and quantify metals associated with different organic species. The same RPLC platform was subsequently coupled with FTMS (Orbitrap and 21T ICRMS) to identify and quantify metalloorganic species by automated identification of chromatographically coherent features that match distinct metal isotopic patterns. Both plant and fungal metal binding metabolites were putatively identified, revealing compound-specific patterns of chelation to biologically essential metals. Numerous plant metabolites, including nicotianamines as well as phytosiderophores typically implicated in iron acquisition by grasses, dominated the speciation of divalent metals such as Ni, Cu, and Zn. In contrast, fungal siderophores bound comparatively more trivalent Fe. These results define direct biochemical pathways that underpin biological-mineral interactions in grassland soils. They also raise new questions about the competition of these compounds for metal binding and their bioavailability to different members of the rhizosphere population.

Poster #H3

The DOE Atmospheric Radiation Measurement (ARM) Climate Research Facility

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The mission of the U.S. Department of Energy Atmospheric Radiation Measurement (ARM) Climate Research Facility, a DOE Office of Science User Facility, is to provide the climate research community with strategically located in situ and remote-sensing observatories designed to improve the understanding and representation, in climate and earth system models, of clouds and aerosols as well as their interactions and coupling with the Earth's surface. ARM operates three fixed atmospheric observatories (in Oklahoma, Alaska, and the Azores), three mobile facilities, and an aerial facility to collect data on cloud, aerosol, and atmospheric processes that impact the Earth's energy balance. In order to provide information to study land-atmosphere interactions and their impact on boundary layer processes, ARM also provides measurements of surface carbon and energy fluxes, soil moisture and temperature profiles, and trace gases at many of its sites. All ARM data is freely available to the scientific community through the ARM archive (<http://www.archive.arm.gov/discovery/>). ARM encourages proposals from the scientific community for deployment of its mobile and aerial facilities, and for field campaign activities at its fixed observatories.

Poster #H4

U.S. Synchrotron Capabilities for Environmental System Science

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Synchrotron X-rays provide the capability to penetrate solid matter and hydrated tissue to study electronic and physical structure at scales ranging from molecular to millimeters. The ability to obtain spatially and temporally resolved molecular fingerprints and mechanistic and dynamic understanding of *in situ* processes within heterogeneous biological and environmental media is enabling unprecedented characterization and imaging of interactions among plants, microbes, and the environment and strongly complement capabilities available at other national user facilities. The Department of Energy's Office of Basic Energy Sciences supports the operation of DOE synchrotron user facilities that enable experiments for studying and understanding structural and functional processes of importance to BER-funded investigators and centers. Within this complex, the Office of Biological and Environmental Research supports technologies, methodologies, and instruments of particular impact in biological and environmental sciences.

The major synchrotrons within the United States that are supported by the DOE provide access via General User proposal systems. These include the Advanced Light Source, the Advanced Photon Source and Stanford Synchrotron Radiation Lightsource. As a result of differing accelerator circumference and energies, each synchrotron provides x-ray beams with general characteristics such as energy range, timing structure, and brilliance, suited to the investigation of specific types of biological and environmental questions and samples. Each offers a range of X-ray based methods through individual experimental stations (beamlines) that optimized for specific types of experiments. Key techniques used by ESS scientists include: i) x-ray absorption spectroscopy to obtain element-specific valence state and molecular structure information; ii) x-ray microscopy to determine spatial distributions of elements, elemental chemistries, and mineralogy in heterogeneous biological and environmental samples; iii) small angle x-ray scattering to determine physical structures and features of nanoparticles, proteins, and thin films; iv) x-ray computed tomography to obtain three-dimensional physical, elemental, and chemical information within opaque media such as soil at nano- to micrometer-scale resolution; and v) x-ray powder diffraction for advanced mineralogical analysis of samples.

We seek to promote and expand collaborations between light sources and the BER research community in order to enable and facilitate fundamental science to understand, predict, manipulate, and design biogeochemical processes. Here we will present information on the facilities and their capabilities, how to access them, and highlights of scientific accomplishments.