2018 Environmental System Science Principal Investigators Meeting

May 1-2, 2018
Bolger Center
Potomac, MD

U.S. DEPARTMENT OF
ENERGY
Office of Science

2018 Environmental System Science Principal Investigators Meeting

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

Terrestrial Ecosystem Science (TES) Program

Program Manager: Dr. Daniel Stover (daniel.stover@science.doe.gov)
Program Website: tes.science.energy.gov/

Subsurface Biogeochemical Research (SBR) Program

Program Managers: Dr. David Lesmes (david.lesmes@science.doe.gov)
Mr. Paul Bayer (paul.bayer@science.doe.gov)
Dr. Amy Swain (amy.swain@science.doe.gov)
Program Website: www.doesbr.org/

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Environmental System Science

Student Abstracts

Poster #1-1

Root Phosphatase Response to Elevated CO_2 is Tree Species Dependent

Kristine Cabugao[1,2,3*], Martijn Slot[4], Jorge Aranda[4], Aurelio Virgo[4], Benjamin Turner[4], Klaus Winter[4], David Weston[2,3], and Richard Norby[2,3]

[1]Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee Knoxville, TN;
[2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN;
[3]Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[4]Smithsonian Tropical Research Institute, Panamá City, Panamá

Contact: cabugaokm@ornl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov

A source of major uncertainty in understanding the global carbon cycle is the response of tropical forests to altered climatic regimes, in particular – the duration and magnitude of the tropical carbon sink. The Next Generation Ecosystem-Experiments – Tropics project is a model- data driven endeavor that focuses on uncovering underlying mechanisms that regulate the exchange of CO_2 between tropical forests and the atmosphere. Decades of research have shown a consistent trend of increasing plant growth with elevated CO_2 – presuming adequate water and nutrients. However, phosphorus is often a limiting nutrient in tropical forests and it is still unclear how phosphorus limitation may constrain responses to elevated CO_2.

A recent modeling study by Yang et al. 2016 showed that phosphorus limitation could constrain NPP under elevated CO_2, suggesting an important role for belowground mechanisms to alleviate phosphorus limitation. In tropical forests, a large amount of phosphorus is locked into organic compounds, which must be mineralized by phosphatase enzymes released from plants and microbes prior to uptake. To improve ecosystem models, root and microbial functions that potentially alleviate P limitation are important to take into account, driving our study to test whether elevated CO_2 does increase phosphatase activity and whether it could be related to root morphological traits, microbial community composition, and leaf functional traits.

In collaboration with the Smithsonian Tropical Research Institute we grew seedlings of four tropical tree species: *Inga spectablis*, *Adenanthera pavonina, Tabebuia rosea, Tabebuia guaycan* in greenhouses at ambient (400 ppm CO_2) or elevated (800 ppm CO_2) conditions for four months. We measured root and soil phosphatase, root morphology, photosynthesis, and we will extract DNA and RNA for microbial community composition and function. Initial ANOVA results with tree species and treatment as factors indicate that response to elevated CO_2 is likely tree species dependent. All tree species except for *I. spectablis* showed increased root specific phosphatase, though individual t-tests show that the elevated CO_2 response was significant only in *A. pavonina* ($p < 0.05$). Plant biomass and total root phosphatase were positively correlated, where the largest plants, which belonged to the tree species *I. spectablis*, also had the highest total phosphatase activity. Further work with this dataset will explore connections between root phosphatase and other root and leaf functional traits to better understand the role of traits in diverging elevated CO_2 response and their possible model implications for the tropical carbon sink.

Poster #21-48

Nonlinear Scaling of Climate Change Impacts in Headwater Catchments: Contribution to Watershed Function Scientific Focus Area

Lauren Foster[1*]

[1]Colorado School of Mines, Golden, CO

Contact: lfoster@mines.edu

BER Program: SBR
Project: LBNL SFA

My role on the Watershed Function Scientific Focus Area (SFA) team is to (1) develop and maintain the hyper-resolution, watershed-scale, physically-based model that nearly every SFA team uses either directly or through comparison to their observations as a tool in their own research; (2) examine how processes scale at different resolutions in order to develop the most appropriate tools for each question; and (3) study the impact of climate changes to water supplies in the East River and whether these impacts are robust across different modeling frameworks.

In 2017, I completed over 50 sensitivity simulations to constrain the parameters that determine flow in the watershed. In the paper for this work a new methodology is presented for downscaling or upscaling hydraulic conductivity parameters in complex mountainous terrain where formal calibration is impossible due to computational limitations. Beyond the need for this work to define the best parameters for the hyper- resolution model used by the team, this work directly contributes to Question 4 of 6 laid out in the SFA 2017 Annual Report: "When and where does fine-scale representation of processes significantly improve prediction of watershed nutrient dynamics, and how can those processes be tractably represented in mechanistic watershed models?" This paper also has implications to the wider research community where continued pushes for higher-resolution, physically-based models at successively larger scales (from full watersheds up to continental scales) require methods to constrain the few parameter sets for subsurface processes.

The parameter work served as the foundation for a climate sensitivity study also completed in Fall 2017. In this work I compare sensitivity to temperature and precipitation across different modeling resolutions to determine how robust climate impact predictions are to different models. The main conclusions from this study are (1) even large increases in precipitation are not enough to compensate for the loss of snowpack, streamflow, and groundwater in a warmer climate and (2) coarse resolution models under-predict reductions to water availability, suggesting that we may need to be more conservative in planning for water scarcity in the Southwest US.

The "Grand Challenge" driving the SFA according to the Annual Report is: "How do mountainous watersheds retain and release water, nutrients, carbon, and metals? How will … [climate] perturbations impact downstream water availability and biogeochemical cycling at decadal to episodic timescales". The hyper-resolution model is a foundation for answering this grand challenge, providing high resolution data in space and time to constrain and contextualize observations across the watershed for the entire team. Beyond my own research, I support other team members in using the models I maintain by gathering forcing datasets for them, answering modeling questions, and improving the README and other files to help people use these modeling tools.

Poster #1-2

Representing Organo-Mineral Associations in Soil Carbon Models: Implications for Carbon Storage and Vulnerability (LBNL TES SFA)

Katerina Georgiou[1*], Rose Z. Abramoff[2], William J. Riley[2], and Margaret S. Torn[2]

[1]University of California, Berkeley, Berkeley, CA
[2]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: kgeorgiou@berkeley.edu

BER Program: TES
Project: LBNL TES SFA

Observed patterns of soil organic carbon (SOC) content across geochemical regimes are signatures of process and provide opportunities to understand the underlying decomposition and stabilization mechanisms that can guide their representation in models. The type of sorption equation used in SOC decomposition models has large implications for SOC stocks and cycling. Here we compared different bulk model formulations of SOC sorption to mineral surfaces, motivated by the myriad of underlying organo-mineral associations, and used laboratory and field incubations to inform model parameters. We explored linear, Langmuir, and Sips adsorption models, where the latter emerges from heterogeneous compositions of substrate and surface components. We show the effect of model representations on predicted trends of SOC as a function of mineralogy and discuss the role of soil C saturation on emergent patterns. Specifically, our results highlight that the response of mineral-associated organic C (MOC) to changes in plant C inputs depends greatly on the C saturation deficit of the soil and thus, the representation of organo-mineral associations in models can lead to nonlinear steady-state responses in MOC. We also find that, consistent with field experiments, the trend in MOC with mineralogy is linear, but, interestingly, the slope depends on the degree of C saturation. We contend that this latter finding is an important consideration for field studies that did not find a universal slope and interpreted this as an inability of mineralogy to explain observed patterns. Our results also suggest that warming affects this slope, with higher temperatures causing a decrease in the amount of MOC for a given saturation capacity and C input rate. This means that more C inputs will be needed to keep the same amount of MOC at higher temperatures. Using field and global data, we infer a MOC saturation capacity for different soil types, which is essential for parameterizing process-based SOC models globally. Organo-mineral interactions play a key role in governing soil C stabilization and long-term storage, and thus, improving their representation for inclusion in Earth system models is crucial for understanding and predicting feedbacks under global change.

Poster #1-3

Digging Deeper: Exometabolomics Reveals Biogeochemical Hotspots with Depth and by Vegetation Type in Arctic Tundra Soils

Mallory P. Ladd[1,3*], Colleen M. Iversen[1,2], Stan D. Wullschleger[2], and Robert L. Hettich[1,3]

[1]Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, Knoxville, TN
[2]Climate Change Science Institute, Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[3]Mass Spectrometry & Laser Spectroscopy Group, Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: laddmp@ornl.gov

BER Program: TES
Project: NGEE-Arctic
Project Website: https://ngee.ornl.gov

With the Arctic warming twice as fast as the rest of the planet, permafrost thaw is increasing both in depth and duration, resulting in increased microbial decomposition of carbon- rich organic matter and the subsequent release of greenhouse gases. Reliably predicting the magnitude of this feedback to the climate system and modeling where and when these carbon- losses are most likely to occur across the landscape requires detailed knowledge of the chemical composition, or decomposability, of soil organic matter—in particular, the water-soluble fraction most available to microbial communities, low molecular weight (LMW) dissolved organic matter (DOM). This soil "exometabolome" represents an information-rich chemical signal of biological activity that is critical to understanding the underlying mechanisms of carbon storage and release in Arctic systems. Due to analytical challenges however (i.e. isolation, detection, quantitation), relatively little is known about how this complex mixture of small molecules varies with soil depth or how it may be influenced by vegetation. We have established a sensitive, high-throughput, and robust workflow from sample collection to analyte annotation, to characterize LMW DOM from soil water samples obtained from polygonal tundra soils near Barrow, Alaska on the Barrow Environmental Observatory (BEO). Soil water extractions were obtained along the length of the organic horizon beneath areas where aboveground vegetation was primarily either *Carex aquatilis* or *Eriophorum angustifolium*, two species commonly found in polygonal tundra systems and of interest to the NGEE-Arctic vegetation team. In evaluating the exometabolomics platform, the median limit of detection was 0.20 ng/mL with linearity over at least two orders of magnitude ($R2 > 0.98$) and reasonable reproducibility (< 15 %) between biological replicates. Untargeted exometabolomic profiling revealed thousands of features present in these soils and showed both positively- and negatively-correlated quantitative trends with depth and between vegetation types. Hundreds of features matched to freely-available, online databases and classes of compounds detected ranged from plant- and microbial metabolites to organic acids, sugars, lipids, and small peptides. Interestingly, although each core represented a single soil horizon (organic) and had similar moisture contents, signature osmolytes that have been linked to desiccation stress were found to accumulate beneath the *Eriophorum* cores, demonstrating the ability of the technique to detect discrete hotspots of biological activity. The optimized approach is sensitive and robust and has enabled a quantitative description of LMW DOM across space in Arctic soils. These data will be leveraged in mechanistic models of microbial decomposition helping to reduce uncertainty in our predictions of how Arctic landscapes will respond under a warmer climate in the future.

Poster #21-35

Effect of Ground Cover on Surface Fluxes of Reactive Nitrogen Oxides at a Disturbed Forest Edge

Zachary C. Payne[1*], Ryan M. Mushinski[2,4], Sally E. Pusede[3], and Jonathan D. Raff[1,4]

[1]Department of Chemistry, Indiana University, Bloomington, IN
[2]Department of Biology, Indiana University, Bloomington, IN
[3]Department of Environmental Sciences, University of Virginia, Charlottesville, VA
[4]School of Public and Environmental Affairs, Indiana University, Bloomington, IN

Contact: zacpayne@indiana.edu

BER Program: SBR
Project: University Award

Reactive oxides of nitrogen, such as nitric oxide (NO), nitrogen dioxide (NO_2), and nitrous acid (HONO), play a crucial role in determining the oxidative capacity of the lower atmosphere. Biogenic emissions of these reactive nitrogen species from terrestrial environments represents as much as half of the total global gaseous nitrogen budget. These emissions are driven by biotic processes related to nitrification and denitrification, or through abiotic reactions of nitrogen oxides on redox-active soil surfaces. Several of these mechanisms have been studied through laboratory studies, however their relative importance in complex environmental matrices can only be realized through field measurements. The objective of this work was to determine the relative importance of biogenic and abiotic processes driving fluxes of NO, NO_2, HONO, and N_2O from soil during a measurement campaign in the summer of 2017 at the Indiana University Research and Teaching Preserve. The site was a disturbed grassy area at the edge of a hardwood forest that is impacted by both anthropogenic and biogenic emissions of NOx. Flux measurements were made using a newly constructed continuous-flow automated chamber array connected to an array of instrumentation, including a newly developed two-wavelength chemiluminescent detector (to quantify NO, NO_2, and HONO) and a cavity ring-down spectrometer (for N_2O measurements). Chambers were placed over bare soil, lightly vegetated, or densely vegetated, as defined by plant biomass. Significant emissions of NO and N_2O were emitted from all soil types during most of the day, whereas NO_2 was consistently deposited to soil; both deposition and emission of HONO was observed over the course of the campaign. Peak emission of NO was roughly two times greater in the bare soil plot than in the densely vegetated plot and tracked solar irradiance. Peak deposition of NO_2 was identical in all three plots and occurred several hours before peak NO emission, suggesting an anthropogenic origin. Aside from temperature and soil moisture, ground coverage had the greatest impact on soil nitrogen emissions, either through plant-microbe competition for soil nitrogen or through light intensity differences associated with shading of normally photoactive soil surfaces.

Poster #1-4

Remote Sensing of Mycorrhizal Distributions

Michala Phillips[1*]

[1]University of California, Riverside, Riverside, CA

Contact: michala.phillips@gmail.com

BER Program: TES
Project: University Award

Terrestrial biosphere models notoriously underestimate the importance and complexity of the carbon (C) land sink. Often these models are limited by the scalability of empirical knowledge about belowground ecosystem processes, specifically regarding the C costs of nutrient acquisition (Shi et. al, 2016). The interplay between C costs and nitrogen (N) acquisition in plants is mediated by symbiotic relationship with mycorrhizal fungi (Terrer et. al, 2016; Shi et. al, 2016). Plant C allocation to mycorrhizal fungi vary and strongly affect N acquisition and differences in mycorrhizal type at the phylum level have significant implications for biogeochemical cycling. Nearly all trees make arbuscular mycorrhizal (AM) or ectomycorrhizal associations (ECM). Plant species that associate with ECM fungi can utilize excess CO_2 resulting in increased biomass without N availability limitations, whereas AM plants are limited in their ability to increase biomass under increased CO_2 by N availability (Terrer et. al, 2016). The incorporation of plant mycorrhizal-identity into terrestrial biosphere models would greatly increase the accuracy of predictions about ecosystem responses to climate change. However, incorporating empirical knowledge about differences between mycorrhizal type into modelling efforts requires a spatial understanding of mycorrhizal distributions. A recent effort by Fisher et al. (2016) made substantial strides classifying forests by mycorrhizal type, through developing a model that links canopy-spectral properties across the plant phenological cycle to plant mycorrhizal identity.

My research builds from the methodology of Fisher et al. 2016, expanding the application from four temperate forests in the U.S. to the global scale. I use reflectance and reflectance derivatives derived from Landsat 8 data coupled with plot level mycorrhizal composition to build global maps of forest mycorrhizal compositions. To do this, I normalize by plant phenology to derive predictor variables aiming to capture six phenological timepoints: leaf flush(T_1), green up (T_2), peak green (T_3), early leaf senescene (T_4), late leaf senescence (T_5), and leaf abscission (T_6). I am building and validate models at the plot level and apply a unified model to entire Landsat scenes. Currently, we have forest inventory analysis (FIA) plot data with percent mycorrhizal type for 38,000 plots across the eastern half of the United States. I am contacting principal investigators for Smithsonian CTFS-ForestGEO network to expand these analyses to the global scale. Both CTFS-ForestGEO and FIA networks, provide massive amounts of forest species composition data collected using a standardized methodology. I am linking the abundance of ground data to Landsat 8 satellite imagery using Google Earth Engine. The products from this research, maps of global mycorrhizal distribution at 30-meter resolution, will be the first to represent plant-mycorrhizal type at this scale with the use of empirical ground data that has not been spatially interpolated. Furthermore, these outputs have the potential to become a widely used data product in terrestrial biosphere models, such as the community land model. The inclusion of this information into modelling efforts will drastically improve the accuracy of our understandings of vegetation responses to increased CO_2 concentrations (Terrer et. al, 2016).

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Poster #1-5

How Topography and its Effects on Fine Root Production Impact Soil Respiration in the Susquehanna-Shale Hills Critical Zone Observatory

Edward Primka IV[1*], Tom Adams[1], Lexie Orr[1], Jason Kaye[1], and David Eissenstat[1]

[1]Pennsylvania State University, University Park, PA

Contact: ejp25@psu.edu

BER Program: TES
Project: University Award

A crucial component of modeling global carbon is an accurate estimation of carbon flux out of forests systems. Soil respiration, which is primarily comprised of heterotrophic and autotrophic respiration, accounts for a large percentage of carbon flux out of a forest system. Of the known components, plant fine roots are considered a main contributor of soil respiration. Furthermore, soil temperature and soil water content are known to impact fine root metabolic rates as well as soil respiration rates. Previous investigations of soil respiration have not taken into account variations of fine root production across topographic gradients within a landscape. We hypothesized that 1) topography across a catchment would shape soil water conditions influencing fine root production and 2) topographic differences would result in differences in soil respiration rate. To test these hypotheses, we collected and analyzed biweekly minirhizotron images and weekly soil respiration data across four topographic regions in the NSF-funded Susquehanna-Shale Hills Critical Zone Observatory (CZO) in central Pennsylvania. Over part of the 2016 growing season, specifically 5/6/16 to 9/30/16, observations were taken from 50 macroplot sites (10 m diameter) with three soil respiration collars and three minirhizotron tubes nested within each macroplot. Macroplot sites were divided into four topographies, specifically ridge top, mid slope planar, swale, and valley floor. Swales refer to concave as opposed to planar midslope locations. Minirhizotron images were collected with a Bartz minirhizotron camera system (Bartz Technology Corp., Carpinteria, CA, USA) in 1 cm increments to a maximum depth of 113 cm in the soil profile. Root production (number of roots/month) was measured on captured images by tracing root growth in Rootfly v2.0.2 (Wells and Birchfield, Clemson University, SC, USA). Soil respiration (μmol/m^2/s), volumetric water content (cm^{3}cm^{-3}) and soil temperature (°C) measurements were taken at each soil collar with a LiCOR 8100 Soil Gas flux system, (LI-COR Biosciences, Lincoln, NE, USA), a Theta Probe model ML2x (Delta-T Devices, Cambridge, UK), and a Taylor 9842 thermometer© respectively. Soil respiration at each topographic location showed a bimodal peak during the growing season. Preliminary analyses suggest that the June peak in respiration was likely caused by fine root production, while the August peak was likely due to soil water and soil temperature. Volumetric water content and soil temperature were not substantially different among topographic locations. Results from this and future analyses will address our hypotheses and improve models of carbon flow through ecosystems at multiple scales.

Poster #21-49

Combining Patch-Scale Modeled Output with Spatial Statistics to Estimate Evapotranspiration Across the Landscape

Joseph Rungee[1*], Anh Tran[2], Boris Faybishenko[2], Susan Hubbard[2]

[1]Sierra Nevada Research Institute, University of California, Merced, CA;
[2]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: jrungee@ucmerced.edu

BER Program: SBR
Project: LBNL SBR SFA
Project Website: watershed.lbl.gov

Difficulty in closing the water balance of a watershed, specifically in mountainous regions, has been sustained for decades despite its importance for downstream water security and environmental maintenance. At the watershed scale, evapotranspiration, ET, can be generalized as $ET = P - Q$, where Q is runoff, and P is precipitation. ET is often considered the most uncertain parameter to quantify, as it is difficult to measure directly, and is generally approximated as a function of potential evapotranspiration. Eddy covariance flux towers provide physical measurements of evapotranspiration, but these towers are relatively new, providing a limited time series, have high installation and maintenance costs, and are few and far between. Physically based models have the capacity to quantify each component of the water balance equation individually with a high spatiotemporal resolution. However, simulations are computationally and time-intensive, and their accuracy strongly depends on model parameterization, which requires accurate spatiotemporal information of the modeled area, calibration and validation. This study will combine patch-scale modeled estimates of ET from the Community Land Model (CLM) with spatial statistics to improve the accuracy and efficiency of ET estimation across the East River watershed, Colorado. More specifically, the CLM model is being used at strategically selected meteorological stations within the watershed to simulate patch-scale ET, which will then be spatially distributed using a suite of readily available spatial data, including, but not limited to, Landsat Normalized Difference Vegetation Index (NDVI), Parameter-elevation Regression on Independent Slopes Model (PRISM) precipitation and temperature, and the National Land Cover Database (NLCD) land-cover product. The results will be initially validated by estimating watershed ET using PRISM precipitation and measured streamflow at a USGS gauge, located at the pour point of the watershed, and then with flux- tower measured ET once available. The questions driving this research include: i) What is the optimal size and number of patches to be modeled to receive good agreement with annual watershed-scale modeled ET?; and ii) How do the statistically based approach and the watershed-scale model compare with ET estimated as the difference of PRISM precipitation and measured streamflow? The proposed approach will provide spatial estimates of ET, improving our ability to more accurately close the water balance, as well as lead to a better understanding of how ET varies with climate extremes, by vegetation type, along an elevational transect, and provide insight for the implications of climate change.

Poster #21-70

Linking Soil Metabolic Potential to Vegetation Type Across Landscape Positions in the East River Watershed, Colorado

Alex Thomas[1*]

[1]University of California, Berkeley, Berkeley, CA

Contact: adthomas@berkeley.edu

BER Program: SBR
Project: LBNL SBR SFA
Project Website: watershed.lbl.gov

Different vegetation types are associated with a suite of different soil edaphic characteristics, nutrient cycling processes, and microbial assemblages and functions. Identifying associations between vegetation types and potential soil microbial functions may be the key to scaling up point observations from microbial ecological studies to watershed processes at kilometer scales. To provide genome-resolved insights into the association between soil microbial functions and vegetation types, we sampled soils at two depths in four different vegetation types (aspen, conifer, meadow, and sagebrush) in nine blocks distributed across the 275 km2 East River watershed in Colorado, USA. These samples collected in 2016 were used for shotgun metagenomic sequencing and to measure soil edaphic characteristics. Over 6 million scaffolds >1kb have been assembled and >100 putative genomes have been preliminary binned. There is evidence that Thaumarchaeota may dominate some soil microbial communities, adding support for this pattern observed in previous genome-resolved studies of soil. In the summer of 2017, 196 samples were collected from four sites to test how soil microbial metabolic potential varies across the growing season. These will be sequenced under a newly awarded Joint Genome Institute Community Science Project award.

Poster #21-61

A Last Line of defense: Understanding Unique Coupled Abiotic/Biotic Processes at Upwelling Groundwater Interface

Chen Wang[1*], Lee Slater[1] and Martin Briggs[2]

[1]Rutgers University-Newark
[2]U.S. Geological Survey

Contact: cw701@scarletmail.rutgers.edu

BER Program: SBR
Project: University Award

Groundwater discharges to streams are critical to surface water quality due to the exchange of heat, gasses, nutrients, and contaminants. Deposition of metal oxides frequently occurs at sediment-water interfaces when groundwater low in dissolved oxygen and high in soluble metal ions mixes with oxygenated surface water. These metal oxides function as a sorption sink for dissolved contaminants (e.g. As, U) due in part to their large surface area. Temporary decreases in dissolved oxygen at the interface can reduce metal oxides and release absorbed contaminants to downstream transport. Therefore, a better understanding of the precipitation and dissolution of metal oxides in sediment-water interface materials is needed to predict contaminant transport through the river corridor. Field characterization at watershed scales necessitates the development of remote sensing methodologies for the comprehensive mapping of groundwater discharge locations, particularly those with high metal oxide content.

Geophysical methods are widely used to characterize the near-surface earth properties as they are non-invasive, high spatial resolution, and time-efficient. There is currently a paucity of benchmark studies regarding how the deposition of metal oxides impacts the electrical and thermal properties of interface sediments. The presence of metal oxides in sediments could potentially 1) increase the ability of electrical current storage when an alternating current is injected; 2) increase the degree of magnetization when a magnetic field is applied and 3) accelerate heat propagation within the sediments. Those three properties can be evaluated by 1) frequency domain phase response acquired from spectral induced polarization (SIP), 2) magnetic susceptibility (MS) and 3) thermal diffusivity, respectively. Along with Dr. Lee Slater, I am leading the thermal and geophysical property analysis on this project based at the East River SFA.

Since Feb 2017, I have collected both lab and field scale geophysical data and have acquired preliminary conclusions guiding then next phase of research at the East River SFA. Lab results show that the occurrence of metal oxides in sediments increase the phase response and MS, which is distinguished from regular sediments. In the 2017 summer field trip to East River, I lead field SIP and MS survey and participated in the other research work including fiber-optic distributed temperature sensing along river, core sampling, self-potential measurements and dye test conducted by our research team. This trip was a great opportunity for me, as all of my previous research had been laboratory-based. Unlike our controlled lab results, the field MS is contaminated by high background noise produced by small magnetite fraction in the parent riverbed sedimentary rocks and failed to detect metal oxides which have a lower MS value. In contrast, SIP is only sensitive to Fe oxides in high content, which was proven to be more reliable than MS for mapping Fe deposition in the field. We will focus SIP survey in the upcoming field trip in the 2018 summer and develop field methodologies to quantitatively characterize the metal oxide distribution in the streambed associated with groundwater discharge zones.

Environmental System Science

Early Career Awards

Poster #9-29

Characterization of Soil Carbon Cycling Across a Tropical Forest Rainfall Gradient for a Dry Down Experiment

Daniela F. Cusack[1*]

[1]University of Los Angeles, Los Angeles, CA

Contact: dcusack@geog.ucla.edu

BER Program: TES
Project: Early Career Research Program

Background/Question/Methods

Soil carbon (C) dynamics in tropical forests remain a large source of uncertainty in Earth system models. Understanding drivers of tropical forest soil C fluxes, including root dynamics and nutrient effects, could greatly improve our ability to predict feedbacks to climate change. We assessed seasonal variation and environmental drivers of soil C pools and CO_2 fluxes for 15 humid tropical forests across rainfall and soil fertility gradients in Panama. Soil respiration was surveyed 4*x* over the wet and dry seasons for one year at each site using four 50-m transects. Air temperature, soil temperature, and soil moisture were measured concurrently with automatic probes. Also, soil C stocks, root biomass, and extractable nutrients were measured for 0 – 100 cm depths at a broader set of 48 sites. These measures serve as baseline data for a rainfall exclusion experiment that is in the construction phase at 6 of the sites across the rainfall gradient. The drying experiment will start during the wet season of 2018 (April).

For baseline data, predictors of soil C stocks and root biomass were assessed across the gradient. For soil CO_2 fluxes, mean annual precipitation (MAP), soil fertility, and time/season were assessed as predictors using repeated measures MANOVA ($n = 4$ time points), using similar analyses for air temperature, soil temperature, and soil moisture. Significant interactions between MAP and time were explored using post-hoc analyses of Wet:Dry season CO_2 flux ratios ($n = 15$), and stepwise models were used to identify predictors of these ratios. Air temperature, soil temperature, and soil moisture were also assessed as predictors of soil CO_2 fluxes ($n = 200$ transects). Statistical significance was $p < 0.05$.

Results/Conclusions

Soil C stocks were weakly related to MAP ($R^2 = 0.11$), and much more of the variation was explained by including root biomass, soil clay content, and extractable base cations in a structural equation model ($R^2 = 0.48$). There were significant effects of seasonality on soil CO2 fluxes, with an interaction between MAP*time. This interaction appeared to be driven by shifts in the magnitude and direction of the seasonal effect at the extremes of the rainfall gradient. In particular, the Wet:Dry season CO_2 flux ratios in the driest sites was 2.25 ± 0.23 (i.e. greater flux during the wet season), versus 0.81 ± 0.09 in the wettest site (i.e. greater flux during the dry season). The best model to predict Wet:Dry season CO_2 flux ratios included soil C, resin phosphorus (P), and extractable potassium (R2 = 0.65), with resin P the strongest univariate predictor ($R^2 = 0.44$). Overall, air temperature, soil temperature, and soil moisture measures together predicted 26% of the variation in soil CO_2 fluxes. These results show significant seasonality in soil respiration across this tropical rainfall gradient, and illustrate that forests with different baseline MAP and soil moisture can have opposite responses to drying. Also, the magnitude of the seasonal shift appeared related to soil phosphorus availability. These results suggest that soil respiration responses to regional drying in tropical forests are likely to vary according to local MAP, and that rock-derived nutrients may provide a control over soil C stocks and fluxes.

Poster #1-27

Contributions of wildland fire to terrestrial ecosystem carbon dynamics in Arctic-Boreal North America from 1990 – 2012

Guangsheng Chen[1], Daniel J. Hayes[2*], and A. David McGuire[3]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]School of Forest Resources, University of Maine, Orono, ME
[3]U.S. Geological Survey, Alaska Cooperative Fish and Wildlife Research Unit, University of Alaska- Fairbanks, Fairbanks, AK

Contact: daniel.j.hayes@maine.edu

BER Program: TES
Project: Early Career Research Program

Burn area and the frequency of extreme fire events have been increasing during recent decades in arctic and boreal ecosystems of North America, and this trend is expected to continue over the 21st century. While many aspects of the North American carbon budget have been intensively studied, the net contribution of fire disturbance to the overall carbon flux at the continental scale remains uncertain. Based on comprehensive, spatially-explicit and long-term fire data, along with the improved model parameterization in a process-based ecosystem model, we simulated the impact of fire disturbance on both direct carbon emissions and net terrestrial ecosystem carbon balance across the Arctic-Boreal region of North America. Based on our synthesis and harmonization of available wildfire databases, more than 5,500 and 20,000 km^2/yr burned on average over the 1990-2012 time period in Alaska and Canada, respectively. Over that time period, fire-caused direct carbon emissions were 18.23±2.74 Tg C/yr in Alaska and 57.87±8.68 Tg C/yr in Canada. However, the net ecosystem carbon balance associated with fire was -10.92 and 11.87 Tg C/yr for Alaska and Canada, respectively, indicating that most of the emitted carbon was re-sequestered by the terrestrial ecosystem. Direct carbon emissions showed an increase in Alaska and Canada during 1990-2012 as compared to prior periods due to more extreme fire events, resulting in a large carbon source from these two regions. Among all continental biomes, the largest carbon source was found to be from the boreal forest, primarily due to large reductions in soil organic matter during, and with slower recovery after, fire events. The interactions between fire and environmental factors reduced the fire-caused ecosystem carbon source. Fire disturbance only caused a weak carbon source as compared to the best- estimate of the terrestrial carbon sink in North America owing to the long-term legacy effects of historical burn area coupled with fast ecosystem recovery during 1990-2012.

Poster #9-4

Applying the FATES Dynamic Vegetation Model to the Western US

Charlie Koven[1*]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: cdkoven@lbl.gov

BER Program: RGCM
Project: Early Career Research Program

In order to understand climate effects on ecosystem structure and composition— and consequent feedbacks to the climate system—in the western US, we must develop and apply process-based dynamic vegetation models that can represent the key processes that govern ecosystem structure. The FATES vegetation model predicts ecosystem structure as an emergent outcome of competition by plants for resources, including water and light. Here we describe initial attempts to apply the FATES model to western US ecosystems, to lay a foundation for understanding climate impacts and feedbacks in the region.

Poster #9-30

Controls over Greenhouse Gas Emissions from Puerto Rican Tropical Rainforest Soils

Melanie A. Mayes,[1*], Ryan K. Quinn,[1] Carla López Lloreda[2], Julia Brenner[1], Jana Phillips[1], Brian Yudkin[2], Debjani Sihi[1], Jianqiu Zheng[1], Christine O'Connell[3], Whendee Silver[3], and Brent Newman[4]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Luquillo Critical Zone Observatory, Rio Grande, PR
[3]Department of Environmental Science, Policy, and Management, University of California, Berkeley, CA
[4]Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM

Contact: mayesma@ornl.gov

BER Program: TES
Project: Early Career Research Program

Wet, tropical ecosystems are responsible for a significant proportion of greenhouse gases into the atmosphere, and a large proportion of tropical gas emissions are due to soil microbial respiration. Landscape position, however, exerts key controls over whether emissions consist of carbon dioxide or methane, and the involvement of terminal electron acceptors ranging from oxygen to sulfate. This poster will summarize a variety of lab- and field-based approaches for understanding greenhouse gas emissions along a 6-point valley to ridgetop transect in the El Yunque National Forest in Puerto Rico. Soils were collected seasonally, characterized, and incubated to quantify carbon dioxide (CO_2) and methane (CH_4) emissions under a variety of moisture conditions, oxygen levels, terminal electron acceptor availability, including nitrate, iron, manganese, and sulfate, and also to capture seasonal variations. Variations in soil moisture changed CO_2 and CH_4 emissions in both valley and ridgetop soils. Valley soils wetted to increase soil moisture content by 25 or 40% emitted more CH4 than control soils, whereas soil dried to decrease moisture content by 25% or 40% did not emit detectable concentrations of CH_4. CO_2 emissions increased in dried valley soils and decreased in wetted valley soils. Ridgetop soils did not emit CH_4 regardless of treatment, but CO_2 emissions increased in wetted treatments and decreased in dried treatments. Incubations on soils collected four times in one year reveal soils are primed based on topographic location to emit either CH_4 or CO_2. Ridgetop soils consistently emitted more CO_2 than valley soils, and never emitted detectable levels of CH_4, unlike valley soils which did emit CH_4 under anaerobic conditions. These results were consistent with field- scale measurements of CH_4 and CO_2 along a valley to ridgetop transect using a Picarro G-2508, in which CH_4 emissions were only observed for valley soils. The addition of terminal electron acceptors to incubation experiments changed CH_4 and CO_2 production rates in both ridgetop and valley soils. Field measurements of soil water were also influenced by topographic position, where nitrate and sulfate disappearance coincided with the appearance of iron and manganese, but only in valley soils. Our work suggests that proportions of greenhouse gas emissions depend on a wide variety of factors, including moisture content, oxygen levels, landscape position, available terminal electron acceptors, and very likely, microbial capabilities. The challenge moving forward will be how to incorporate the information into a model that improves representation of greenhouse gas emissions while representing complexities in landscape position, moisture, and time.

Poster #9-31

Incorporation Of "Omics" Information into a Soil Biogeochemical Model: A Novel Model Scheme to Regulate Microbial Functions and Soil Carbon Dynamics in Response to Environmental Change

Yang Song[1*], Qiuming Yao,[2] Gangsheng Wang[1], Xiaojuan Yang[1], Chongle Pan[2], Benjamin L. Turner[3], S. Joseph Wright[3], Eric R. Johnston[4], Minjae Kim[4], Kostas Konstantinidis[4], Malak M. Tfaily[5], Ljiljana Pasa-Tolic[5], and Melanie A. Mayes[1]

[1]Environmental Sciences Division & Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Computer Science and Mathematics Division, Oak Ridge National Lab, Oak Ridge, TN
[3]Smithsonian Tropical Research Institute, Balboa, Ancon, Republic of Panama
[4]School of Civil and Environmental Engineering, Georgia Technological University, Atlanta, GA
[5]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA.

Contact: songy1@ornl.gov

BER Program: TES
Project: Early Career Research Program (Melanie Mayes)

Both observations and modeling studies show large uncertainties in feedback between soil carbon and climate change. This uncertainty mainly stems from our limited understanding of the soil microbial community, in terms of its diverse structure, function, and capacity to adapt to environmental change. The advent of "omics" technology is revolutionizing our ability to understand the microbial community. Metagenomics analysis of soil samples from both phosphorus (P) -deficient and P-fertilized sites in Panama demonstrated that community-level enzyme functions can adapt to maximize the acquisition of P and minimize energy demand for foraging. This optimization of foraging can mitigate the imbalance of the C/P ratio between soil substrates and the microbial community, thereby relieving nutrient limitations on microbial CO_2 emissions. Incorporation of microbial dynamics into biogeochemical models remains challenging due to the difficulty in quantitatively parameterizing omics-based information. This study introduces the concept of the soil "enzyme function group" to parameterize omics-informed functions of the microbial community in the Continuum Microbial Enzyme Decomposition model (CoMEND).

In the CoMEND model, the chemical composition of soil organic matter (SOM) pools was based on data generated using Fourier transform ion cyclotron resonance mass spectrometry (i.e. C-rich SOM, N-rich SOM and P-rich SOM) and the degree of depolymerization. The enzyme functional groups that catalyze the SOM pools are quantified by the relative composition of gene copy numbers. The responses of microbial activities and SOM decomposition to nutrient and water availability are simulated by optimizing the allocation of enzyme functional groups to maximize P acquisition and minimize energy demand. The model is able to reproduce lab- and field-scale observations, including higher microbial biomass in field samples of P-fertilized soils, higher CO_2 production in lab-scale incubation experiments using P-fertilized soils, and seasonal variability in microbial biomass with wet and dry season alternation in tropical soils. Therefore, the omics-informed dynamic enzyme allocation in the CoMEND model enables us to capture varying microbial activity and soil carbon dynamics in response to shifting nutrient and water constraints over time in Panama soils.

Poster #9-32

Soil Carbon Storage and Turnover in Tropical Forests Along a Precipitation Gradient in Panama

Kari Finstad[1*], Lee Dietterich[2], Daniela Cusack[2], Zina Zhang[1], Benjamin Turner[3], and Karis McFarlane[1]

[1]Center for Accelerator Mass Spectrometry, Lawrence Livermore National Laboratory, Livermore, CA
[2]Department of Geography, University of California, Los Angeles, Los Angeles, CA
[3]Smithsonian Tropical Research Institute, Panama

Contact: mcfarlane3@llnl.gov

BER Program: TES
Project: Early Career Research Program

Tropical forests account for over 50% of the global terrestrial carbon sink and 29% of global soil carbon, but the stability of carbon in these ecosystems under a changing climate is unknown. Recent work suggests moisture may be more important than temperature in driving soil carbon storage and emissions in the tropics. Here, we explore the role of moisture and soil type in controlling soil carbon storage and turnover at a natural precipitation gradient in Panama where differences in parent material result in different fertility and other soil characteristics. While the three sites included in this study maintain similar mean annual temperature, they range in mean annual precipitation from 1875 to 2850 mm/yr. At each precipitation level (low, medium, high), a high and a low fertility soil were also compared. Surface soils were incubated to determine the size of the "active" carbon pool and the age of heterotrophic respiration. Bulk soil carbon stocks and radiocarbon values were also measured and compared to land model predictions.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Poster #9-34

Tropical Forest Response to a Drier Future: Measurement and Modeling of Soil Organic Matter Stocks and Turnover

Karis McFarlane[1*], Kari Finstad[1], Ashley Campbell[1], Charlie Koven[2], Jennifer Pett-Ridge[1], Jennifer Powers[3], Oliver van Straaten[4], Ben Turner[5], Edzo Veldkamp[4], and Nina Zhang[1]

[1]Lawrence Livermore National Laboratory, Livermore, CA
[2]Lawrence Berkeley National Laboratory, Berkeley, CA
[3]University of Minnesota, Minneapolis, MN
[4]University of Göttingen, Göttingen, Germany
[5]Smithsonian Tropical Research Institute, Pamama

Contact: mcfarlane3@llnl.gov

BER Program: TES
Project: Early Career Research Program

Tropical forests account for over 50% of the global terrestrial carbon sink and 29% of global soil carbon, but the stability of carbon in these ecosystems under a changing climate is unknown. Recent work suggests moisture may be more important than temperature in driving soil carbon storage and emissions in the tropics. However, data on belowground carbon cycling in the tropics is sparse, and the role of moisture on soil carbon dynamics is underrepresented in current land surface models limiting our ability to extrapolate from field experiments to the entire region. We measured radiocarbon (^{14}C) and calculated turnover rates of organic matter from 37 soil profiles from the Neotropics including sites in Mexico, Brazil, Costa Rica, Puerto Rico, and Peru. Our sites represent a large range of moisture, spanning 710 to 4200 mm of mean annual precipitation, and include Andisols, Oxisols, Inceptisols, and Ultisols. We compared measured soil C stocks and ^{14}C profiles to data generated from the Community Land Model (CLM) v.4.5 and have begun to generate data from the E3SM Land Model v.1. We found a large range in soil ^{14}C profiles between sites, and in some locations, we also found a large spatial variation within a site. We found that modeled carbon stocks were consistently higher than measured stocks, modeled soil carbon ages were older than measured values near the surface (upper 50 cm), and that modeled soil carbon ages for deep soil carbon were younger than measured deep soil carbon ages. Additionally, the models did not capture the variation in ^{14}C and C stock profiles that we observed in measured soil carbon profiles between and within the sites across the Neotropics.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-736060.

Poster #1-28

Rain Increases Methane Production and Methane Oxidation in a Boreal Thermokarst Bog

Rebecca B Neumann[1*], Colby J Moorberg[1,2], Jesse C Turner[1], Andrea Wong[1] Mark P Waldrop[3], Eugenie Euskirchen[4], Colin Edgar[4], and Merritt R Turetsky[5]

[1]University of Washington, Seattle, WA
[2]Kansas State University, Manhattan, KS
[3]United States Geological Survey, Menlo Park, CA
[4]University of Alaska Fairbanks, Fairbanks, AK
[5]University of Guelph, Guelph, Ontario, Canada

Contact: rbneum@uw.edu

BER Program: TES
Project: Early Career Research Program
Project Website: https://www.uwhydrobiogeochem.com/plants-wetland-methane/

Bottom-up biogeochemical models of wetland methane emissions simulate the response of methane production, oxidation and transport to wetland conditions and environmental forcings. One reason for mismatches between bottom-up and top-down estimates of emissions is incomplete knowledge of factors and processes that control microbial rates and methane transport. To advance mechanistic understanding of wetland methane emissions, we conducted a multi-year field investigation and plant manipulation experiment in a thermokarst bog located near Fairbanks, Alaska. The edge of the bog is experiencing active permafrost thaw, while the center of the bog thawed 50 to 100 years ago. Our study, which captured both an average year and two of the wettest years on record, revealed how rain interacts with vascular vegetation and recently thawed permafrost to affect methane emissions.

In the floating bog, rain water warmed and oxygenated the subsurface, but did not alter soil saturation. The warmer peat temperatures increased both microbial methane production and plant productivity at the edge of the bog near the actively thawing margin, but minimally altered microbial and plant activity in the center of the bog. These responses indicate processes at the edge of the bog were temperature limited while those in the center were not. The compounding effect of increased microbial activity and plant productivity at the edge of the bog doubled methane emissions from treatments with vascular vegetation during rainy years. In contrast, methane emissions from vegetated treatments in the center of the bog did not change with rain. The oxygenating influence of rain facilitated greater methane oxidation in treatments without vascular vegetation, which offset warming-induced increases in methane production at the edge of the bog and decreased methane emissions in the center of the bog.

These results elucidate the complex and spatially variable response of methane production and oxidation in thermokarst bogs to energy and oxygen inputs from rain, and have implications for how boreal 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 bottom-up wetland methane models.

Poster #XXX

Ammonia-Oxidizing Archaea are the Dominate Nitrifiers in Two Midwestern (USA) Forest Types, But Do Not Contribute to Nitric Oxide Production

Ryan M. Mushinski[1, 4], Zachary C. Payne[2.4], Douglas B. Rusch, [5] Jeffrey R. White[3.4], Richard P. Phillips[1], and Jonathan D. Raff[1.2.4]

[1]Department of Biology, Indiana University, Bloomington, IN
[2]Department of Chemistry, Indiana University, Bloomington, IN
[3]Integrated Program in the Environment, Indiana University, Bloomington, IN
[4]School of Public and Environmental Affairs, Indiana University, Bloomington, IN
[5]Center for Genomics and Bioinformatics, Indiana University, Bloomington, IN

Contact: jdraff@indiana.edu

BER Program: SBR
Project: Early Career Research Program

In terrestrial ecosystems, nitrification plays a crucial role in regulating the overall abundance of oxidized inorganic nitrogen and is responsible for initiating the subsequent loss of soil nitrogen (N) via volatilization and leaching. Gross production of nitrate (NO_3^-) is limited by ammonia-oxidation, which is defined as the microbiological oxidation of ammonia (NH_3) to nitrite (NO_2^-)via intermediates. This process is mediated by both ammonia-oxidizing archaea (AOA) and bacteria (AOB). In many soils, AOA greatly outnumber AOB indicating their potential importance to rates of nitrification, especially in acidic soils where AOA tend to dominate. Gaseous by-products of ammonia-oxidation include nitric oxide (NO), which, if not consumed by other processes, can be released from the soil and contribute to the greenhouse effect. In this study, we evaluated the abundance and N-cycle activity of AOA and AOB in two different mixed hardwood stand-types typically found throughout the Midwestern USA. Stand-type differentiation was based on whether plots were either dominated by trees that associate with arbuscular mycorrhizal fungi (AM) or ectomycorrhizal fungi (ECM). In general, AM plots possessed more labile litter and higher rates of net nitrification. Both stand-types possessed acid soil; however, ECM soil was more acidic. The abundance of AOA and AOB, based on qPCR assays, illustrated that AOA were roughly 2X more abundant than AOB in AM stands and 5X more abundant in ECM stands. We used an inhibitor-based nitrification assay (1-octyne) to determine that in AM soil, AOA contributed 80% to the net production of NO_3. Additionally ECM stands showed no observable net nitrification; however, the addition of a known total-nitrification inhibitor (acetylene) resulted in accumulation of NH_3, which was equivalent to the AM stands, indicating that ammonia oxidization was occurring in ECM stands. Nitrification-derived nitric oxide (NO) flux was measured from soil using an aerobic continuous-flow soil incubation system connected to a chemiluminescence detector. Soil from AM stands produced significantly more NO relative to the ECM stands. The application of nitrification inhibitors indicated that AOA did not contribute to the efflux of NO, which may be a function of their utilization of NO as a nitrification intermediate. This work illustrates that (1) AOA may be the dominant ammonia-oxidizing taxa in Midwestern mixed-hardwood forest soils, (2) AM and ECM stands are functionally different in the production of NO, and (3) AOA do not contribute to NO fluxes from soil, indicating a stark difference from functionally similar microbes, AOB.

Poster #XXX

Hydrology, Sediment or Permafrost: Why Do High Latitude Rivers Move So Slowly?

Joel Rowland[1], Jordan Muss[2], Eitan Shelef[3], Sophie Stauffer[1], and Daniel Ahrens[4]

[1]Earth & Environmental Science Division, Los Alamos National Laboratory, Los Alamos, NM
[2]Commonwealth Computer Research, Inc., Charlottesville, VA
[3]Department of Geology & Environmental Science, University of Pittsburgh, Pittsburgh, PA
[4]University of California-Berkeley, Berkeley, CA

Contact: jrowland@lanl.gov

BER Program: SBR
Project: Early Career Research Program

Due to climatic conditions, high latitudes have unique land surface properties and hydrology. Up to 24% of the northern hemisphere is underlain by permafrost. The presence of frozen soils strongly controls hydrological responses such as infiltration and runoff. Most high latitude rivers and streams exhibit nival hydrological regimes with snow dominated spring floods, flow limited to a fraction of the year, and ice cover during winter and spring months. Additionally, frozen soils and ground ice lead to thermally mediated erosion and creep processes. Even though three out of the 10 largest (by drainage area) rivers on earth flow across watersheds underlain by permafrost, there has, to date, been no systematic examination river erosion rates in these environments. With low sediment production rates in arctic landscapes, bank erosion in these systems is a major source of sediment to rivers and heavily influences the exchange of carbon from permafrost-dominated floodplains to rivers and oceans. We measured up to four decades of bank erosion rates on over 5,000 km of high latitude rivers using satellite imagery and aerial photography. Comparing these results to our newly assembled global compilation of published erosion rates, we find that erosion rates of high latitude rivers are significantly lower than rates on lower latitude rivers. To explain this systematic difference in erosion rates, we explore the possible influences of high latitude hydrology, sediment loads, and permafrost on bank erosion rates and river migration. Based on field studies, we also explore how permafrost, ice break up, bank grain size, and hydrology influence both spatial and temporal variability in erosion rates along both a small meandering (Selawik) and a large multi-threaded (Yukon) river in Alaska. Our results highlight the sensitivity of high-latitude rivers to both changes in Arctic hydrology and temperatures. Alterations in river bank erosion will likely alter both the magnitude and composition of sediment, nutrients and carbon that are release from the land to rivers and the ocean.

Poster #1-29

Awakening the Sleeping Giant: Multi-omics Enabled Quantification of Microbial Controls on Biogeochemical Cycles in Permafrost Ecosystems

Neslihan Taş[1*]

[1]EESA, Lawrence Berkeley National Laboratory, Berkeley, CA

BER Program: Genomics Sciences Program
Project: Early Career Research Program

Arctic soils store large amounts of biomass and water from warmer periods in the history of the Earth that became preserved in permafrost during cooling and glaciation events. Permafrost soils contain a broad diversity of cold-adapted microbes, whose metabolic activity depends on environmental factors such as temperature changes that cause cycles of freezing and thawing in the soil. Permafrost defines just the thermal state of soil, meaning the soil's hydrology, physics and chemistry can differ vastly among locations. Microbial metabolism leads to decomposition of soil organic matter, substantially impacting the cycling of nutrients and significantly affecting the arctic landscape. However, the relationship between permafrost microbial properties and biogeochemical cycles is poorly understood. Ribosomal gene surveys have demonstrated dramatic differences in permafrost microbiome structure across the entire Arctic region, although the causes or the consequences of these differences are unknown. Emerging metagenomic studies are uncovering the extent and depth of the permafrost genetic reservoir. Using cutting-edge multi-omic approaches, this project studies the functional and phylogenetic evolution of permafrost microbial communities during thaw across multiple arctic locations. This project uses field experiments, laboratory manipulations, and multi-omics approaches to examine how microbial processes, biogeochemical transformations, and hydrology interact during permafrost thaw in different sites in Alaska in order to determine how these factors drive biogeochemical cycles in different Arctic soils.

This research is supported by DOE Early Career Program by the Office of Biological and Environmental Research in the DOE Office of Science.

Poster #XXX

Computational Bayesian Framework for Quantification of Predictive Uncertainty in Environmental Modeling

Ming Ye[1*]

[1]Department of Earth, Ocean, and Atmospheric Science, Florida State University, Tallahassee, FL

Contact: mye@fsu.edu

BER Program: SBR
Project: Early Career Research Program

A computational Bayesian framework has been developed for quantification and reduction of uncertainty in environmental modeling. In this year of the project, we have collaborated with scientists at the Oak Ridge National Laboratory (ORNL) and Pacific Northwest National Laboratory to apply our computational methods to several problems of interest to DOE. The collaboration with Xingyuan Chen at PNNL is focused on developing a Bayesian network that can incorporate uncertainty in model parameters, structures, and scenarios in a flexible manner. This Bayesian network has been used for a sensitivity analysis to determine important model parameters and processes at the 300 Area of the Hanford Site. The collaboration with the ORNL is for mercury modeling and for leaf modeling. The collaborative research with Scott Brooks at ORNL on mercury modeling has produced a model that integrates the mercury complexation model (WHAM Model VII) into the PHREEQC framework. The on-going research is to use the PHREEQC VII model for addressing uncertainty in equilibrium coefficients of mercury reactions. Different ways of addressing the parametric uncertainty reported in literature are compared to explore the appropriate way of addressing the uncertainty. The collaborative research with Anthony Walker at ORNL on leaf modeling is to integrate our research of multi- models sensitivity analysis and his multi-hypotheses leaf photosynthesis modeling, and the goal is to identify the processes important to leaf photosynthesis. Our contribution is to develop a theoretical framework for the identification. A computationally efficient method has been developed for implementing the framework.

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 have evaluated several state-of-the-art methods for evaluating the Bayesian evidence, and they are the thermodynamics integration, stepping-stone, and nested sampling methods. Our research of this year is focused on the nested sampling method by improving its sampling efficiency. 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. We plan to develop a public domain software so that our computational methods can be used by other scientists who may not be an experts on computational science but are interested in exploring model structure uncertainty.

Terrestrial Ecosystem Science

University Awards

Poster #1-74

Aerodynamic Canopy Height: A Simple Metric for Temporal Dynamics of Canopy Heights Derived with Eddy Covariance Momentum Data Collected Across North American Flux Networks

Housen Chu[1,2*], Dennis D Baldocchi[1], Cristina Poindexter[3], Michael Abraha[4], and AmeriFlux Contributors

[1]University of California-Berkeley, Berkeley, CA
[3]California State University, Sacramento, CA
[4]Michigan State University, East Lansing, MI

Contact: baldocchi@berkeley.edu

BER Program: TES
Project: University Award

The networks of eddy covariance tower sites (e.g., AmeriFlux, European Flux Networks, AsiaFlux) have collected ~10^8 hours of momentum flux and wind statistics data worldwide. We present the first synthesis utilizing this abundant data set and demonstrate how a simple flux-derived metric— aerodynamic canopy height—can be calculated and used to infer the variation of canopy heights from site to site and from time to time. Testing across 74 forest sites from the North American flux networks (~550 site-years), we show the robustness of aerodynamic canopy heights in capturing the site-to-site difference across a wide range of forest canopy heights (~1 to ~60 m). With caution, the yearly estimates could potentially be used for detecting long-term growing trends or structural changes at forest sites. At 23 cropland and grassland sites (~94 site-years), we show that the weekly aerodynamic canopy heights captured the canopy dynamics over the course of growing seasons across the majority of tested years. This suggests that aerodynamic canopy height could serve as an independent approach for tracking the seasonal dynamics of vegetation canopy, and be used to validate next generation satellite LiDAR measurements. Given the amount of momentum flux data collected and the diversity of vegetation covered by the flux networks, the flux-derived canopy heights have great potential for a variety of further applications and research.

Poster #9-40

Near Surface Measurement of Solar Induced Chlorophyll Fluorescence in Amazonia

Berry, J.[1*]

[1]Carnegie Institution for Science, Stanford, CA

Contact: jberry@carnegiescience.edu

BER Program: TES
Project: University Award

Abstract Coming soon

Poster #9-36

Amazon Gross Primary Production Inferred at Regional Scale from Satellite Carbonyl Sulfide Retrievals

Campbell J.E.[1*], Stinecipher[1], J. Berry J.A.[2], Whelan, M.[1], Domingues T.F.[3], Manzi A.O.[4], Maseyk K.[5], and Seibt U.[5]

[1]University of California, Santa Cruz, Santa Cruz, CA
[2]Carnegie Institute for Science, Stanford University, Stanford, CA
[3]University of São Paulo
[4]Instituto Nacional de Pesquisa Amazônicas
[5]University of California, Los Angeles, Los Angeles, CA

Contact: elliott.campbell@ucsc.edu

BER Program: TES
Project: University Award

Correctly predicting the magnitude of tropical gross primary production (GPP) is critical for carbon cycle modeling, but poorly constrained at regional scales. One promising approach is the use of atmospheric carbonyl sulfide (OCS) uptake as a proxy for regional GPP. Here, we simulate carbonyl sulfide concentrations with an atmospheric chemical transport model, driven by a variety of surface flux scenarios encompassing a wide range of model GPP estimates for the Amazon basin. We compare the model output to satellite OCS measurements in order to arrive at a regional estimate of annual GPP that is near the low extreme of the model ensemble range. This OCS-based estimate is consistent with independent constraints from solar-induced fluorescence and eddy flux tower upscaling, while incorporating the benefits of temporal and spatial integration.

Poster #9-36

Tropical Response to Altered Climate Experiment (TRACE): How Plant-Soil Interactions Both Respond To and Help Dictate Lowland Tropical Forest Responses To Warming

Molly Cavaleri[1*], Sasha Reed[2], Eoin Brodie[3], and Tana Wood[4]

[1]Michigan Technological University, Houghton, MI;
[2]U.S. Geological Survey, Moab, UT;
[3]Lawrence Berkeley National Laboratory, Berkeley, CA;
[4]USDA Forest Service, Luquillo, Puerto Rico

Contact: macavale@mtu.edu

BER Program: TES
Project: University Award
Project Website: forestwarming.org

Due to the enormous amount of carbon, water, and energy tropical forests exchange with the atmosphere, there is substantial interest in refining our understanding of how these forests will respond to environmental changes such as a warming climate. While a high level of biodiversity suggests the potential for ecosystem-level resilience to increasing temperature, the data that do exist suggest that lowland tropical forests may indeed by quite sensitive to even subtle changes in temperature due to (1) already warm temperatures and (2) organisms that evolved and developed with low diurnal, seasonal, and interannual temperature variation. Here we describe a novel lowland tropical forest warming experiment in Puerto Rico where we used infrared warming lamps to heat understory plants and soils, as well as canopy warming infrastructure, to explore the relationships between temperature, plant physiology, soil respiration and fertility, and the biogeochemical exchanges that connect these ecosystem components. We found that tropical forest plants and soils were quite responsive to changes in temperature and that multiple carbon pools and fluxes were affected. Both foliar and root respiration acclimated to warmer conditions, though photosynthesis showed signs of stress and only partial acclimation. Availability of soil nutrients were also affected by warming. For example, indices of phosphorus availability declined with warming, suggesting that increased temperatures could indirectly affect tropical rain forest function above and belowground via changes to the availability of key nutrients. Further, warming stimulated soil CO_2 rates and suggested that, at least over the short-term, plant reductions in CO_2 uptake could be coupled with soil increases in CO_2 loss. We will synthesize our current understanding of the patterns and implications we've observed in the first year of warming for this unique tropical forest field experiment. We will explicitly consider above- and belowground processes, as well as their interactions. 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 #1-66

Theoretical and Empirical Support that Plant Roots Stimulate the Decomposition of Protected, But Not Unprotected, Soil Carbon

Jessica A. M. Moore[1], Benjamin N. Sulman[2], Melanie A. Mayes[3], and Aimée T. Classen[4]

[1]Department of Ecology & Evolutionary Biology, University of Tennessee, Knoxville, TN
[2]Program in Atmospheric and Oceanic Sciences, Princeton University, Princeton, NJ
[3]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[4]The Rubenstein School of Environment & Natural Resources, University of Vermont, Burlington, VT

Contact: Aimee.Classen@uvm.edu

BER Program: TES
Project: University Award

Roots release carbon (C) into soil where it is consumed by microbes and then released as CO_2 or stabilized in soil, thus altering soil C pools. We hypothesized that root inputs increase decomposition of soil C, and we expected decomposition of soil C that is protected from microbes to be more sensitive to root inputs than unprotected soil C. We quantified how root inputs affect soil C decomposition using a rhizosphere C model − Carbon, Organisms, Rhizosphere, and Protection in the Soil Environment model (CORPSE) − and a field experiment that manipulated root density. We empirically tracked decomposition of two isotopically labeled substrates that differed in their energetic demands for decomposition, leaf material and starch. Protected C decomposition in CORPSE increased with root inputs, and leaf material decomposition in the field study increased with root density. Unprotected C decomposition in CORPSE and starch decomposition in the field study were unchanged by root inputs. Microbial biomass and beta-glucosidase activity increased with root inputs. Root-microbe interactions affected pools of C differently via changes in microbial biomass and enzyme activity. Protected C decomposition was sensitive to root inputs while unprotected C decomposition was not. Environmental changes influencing root-microbe interactions could, therefore, alter soil C stocks and biogeochemical cycling.

Poster #1-67

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

Xiao-Jun Allen Liu[1], Serita D. Frey[2], Ken M. Kemner[3], Jerry M. Melillo[4], Bhoopesh Mishra[5], and Kristen M. DeAngelis[1*]

[1]University of Massachusetts-Amherst, Amherst, MA
[2]University of New Hampshire, Durham, NH
[3]Argonne National Laboratory, Argonne, IL
[4]Marine Biological Laboratory, Woods Hole, MA
[5]Illinois Institute of Technology, Chicago, IL

Contact: deangelis@microbio.umass.edu

BER Program: TES
Project: University Award

Warming accelerates the decomposition of stored carbon (C) in soils, though long-term trends suggest that this effect extends beyond a kinetic response. Microbial C use efficiency (CUE) and the dynamic nature of physical protection of soil organic matter (SOM) have emerged as control points in the temperature sensitivity of microbial feedbacks to climate. In a field experiment at the Harvard Forest in Massachusetts, where soils have been exposed to 27 years of warming at 5 °C above ambient, periods of soil C degradation have been punctuated by periods of changes in soil microbial dynamics. While long-term warming has caused the soil system to act as a positive feedback to climate, our studies show microbes acting to promote negative feedbacks to climate. We hypothesize that long-term warming has altered the mineral association of SOM such that soil C in heated plots is less physically protected and more vulnerable to microbial degradation and subsequent mineralization to CO_2. Further, we hypothesize that microbial efficiency of complex SOM utilization (*e.g.*, requiring considerable extracellular degradation) is decreasing, which may account for the large loss of soil C over time. Soils were collected from the long-term warming study and macroaggregates and microaggregates (250 – 2000 and < 250 µm) were isolated. Two short-term incubations were conducted (1) with glucose, cellobiose and cellulose, and (2) with intact and crushed aggregates. Compared to macroaggregates, microaggregates had greater soil nitrogen, microbial biomass C (MBC), dissolved organic C (DOC), DNA content, consistent with the idea that SOM is more physically protected in microaggregates than in macroaggregates. Using metabolic quotient as a proxy for CUE, measured as the respiration CO_2-C produced per unit of microbial biomass, we find that microaggregates have a smaller metabolic quotient, indicating a higher CUE compared to macroaggregates. Soil microbial DNA was labeled with heavy water ($H_2{}^{18}O$, 97 atom%) and will be analyzed to determine how long-term warming affects CUE for different aggregate sizes. To understand how bulk C chemistry of soils changes due to long- term warming, X-Ray Raman scattering measurements were conducted at sector 20-ID of APS. C signal of the measured samples suffers from low signal to noise ratio due to high background from soil mineral content, making it difficult to analyze the samples meaningfully and quantify the differences. These experiments would serve as a justification for beam time at European Synchrotron Research Facility in Grenoble, France where samples could be measured at an energy (6 KeV) below the excitation energy for Fe (7.2KeV) using 72 detectors as opposed to 19 at APS. This approach will likely 1) reduce background from mineral content in the soil and 2) improve statistics significantly due to four-fold improvement in detection capability. Once quantified, the contributions of CUE and physical protection to C cycling can be incorporated into the MIMICS model, which can then be slotted into the decomposition module of our global biogeochemical model, the Terrestrial Ecosystem Model (TEM). 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 of 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 #1-59

Using a Spatially-Distributed Hydrologic Biogeochemistry Model with Nitrogen Transport to Study the Spatial Variation of Carbon Stocks and Fluxes in a Critical Zone Observatory

Yuning Shi[1], David Eissenstat[1], Yuting He[2], and Kenneth Davis[2]

[1]Department of Ecosystem Science and Management, Pennsylvania State University, State College, PA
[2]Department of Meteorology and Atmospheric Science, Pennsylvania State University, State College, PA

Contact: dme9@psu.edu

BER Program: TES
Project: University Award

Most current biogeochemical models are 1-D and represent one point in space. Therefore, they cannot resolve topographically driven land surface heterogeneity (e.g., lateral water flow, soil moisture, soil temperature, solar radiation) or the spatial pattern of nutrient availability. A spatially distributed forest biogeochemical model with nitrogen transport, Flux-PIHM-BGC, has been developed by coupling a 1-D mechanistic biogeochemical model Biome-BGC (BBGC) with a spatially distributed land surface hydrologic model, Flux-PIHM, and adding an advection dominated nitrogen transport module. Flux-PIHM is a coupled physically based model, which incorporates a land-surface scheme into the Penn State Integrated Hydrologic Model (PIHM). The land surface scheme is adapted from the Noah land surface model, and is augmented by adding a topographic solar radiation module. Flux-PIHM is able to represent the link between groundwater and the surface energy balance, as well as land surface heterogeneities caused by topography. In the coupled Flux-PIHM-BGC model, each Flux-PIHM model grid couples a 1-D BBGC model, while nitrogen is transported among model grids via surface and subsurface water flow. In each grid, Flux-PIHM provides BBGC with soil moisture, soil temperature, and solar radiation, while BBGC provides Flux-PIHM with spatially-distributed leaf area index.

The coupled Flux-PIHM-BGC model has been implemented at the Susquehanna/Shale Hills Critical Zone Observatory. The model-predicted aboveground vegetation carbon and soil carbon distributions generally agree with the macro patterns observed within the watershed. Predicted watershed average vegetation carbon and soil carbon storage also agree well with observations. The importance of abiotic variables (including soil moisture, soil temperature, solar radiation, and soil mineral nitrogen) in predicting aboveground carbon distribution is calculated using a random forest. The result suggests that the spatial pattern of aboveground carbon is controlled by the distribution of soil mineral nitrogen. A Flux-PIHM-BGC simulation without the nitrogen transport module is also executed. The model without nitrogen transport fails in predicting the spatial patterns of vegetation carbon, which indicates the importance of having a nitrogen transport module in spatially distributed ecohydrologic modeling.

Poster #1-52

Effects of Experimental Warming & Elevated CO_2 on Trace Gas Emissions from a Northern Minnesota Black Spruce Peatland

Adrien C. Finzi[1*], Allison L. Gill[1,2], I-Fang Hsieh[1], and Marc-André Giasson[1]

[1]Boston University, Boston MA;
[2]Unniversity of Minnesota, St. Paul, MN

Contact: afinzi@bu.edu

BER Program: TES
Project: University

High latitude peatlands represent a particularly significant terrestrial carbon sink, containing nearly half of the soil carbon pool on Earth. 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. The magnitude of forms of these C losses as CO2 and CH4 remains highly uncertain. To address these uncertainties, this project uses a measurement and modeling campaign at the DOE-funded *Spruce and Peatland Responses Under Changing Environments* (SPRUCE) experiment in the Marcell Experimental Forest, MN. The objectives of the research are intended to bridge a gap between data and models for policy-relevant outcomes by:

1. making high-precision, high-temporal resolution measurements of the flux and ^{13}C-isotopic composition of CO_2 and CH_4 from a boreal, black spruce peatland exposed to high concentrations of atmospheric CO_2 and experimental warming up to 9^oC;
2. testing fundamental hypotheses regarding the effects of warming and elevated CO_2 on C-based greenhouse gas efflux in a peatland ecosystem; and
3. expanding and testing *a soil process model of O_2, CO_2, and CH_4 production and consumption guided by formal data-model assimilation* and using a novel, parsimonious, statistical representation of redox conditions across populations of soil microsites that *could be incorporated into larger EESMs*;

By utilizing a "*systems approach*" this research "s*eeks to improve the representation of these integrated processes in coupled models"* by further developing a belowground terrestrial-aquatic interface, process-based model with the specific goal of using a model structure that could be integrated with larger ecosystem and global models (Sihi et al., 2018). This project directly addresses the TES's interest in Terrestrial-Aquatic Interfaces. The proposed ModEx framework is central to "*understanding of the roles of Earth's biogeochemical systems*" at decadal to centennial time scales, a centerpiece of the Office of Biological & Environmental Research mission.

Poster #1-53

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

Joshua B. Fisher[1*], Richard P. Phillips[2], Edward R. Brzostek[3], Tom Evans[4], Kara Allen[3], and Michala L. Phillips[5]

[1]University of California, Los Angeles, Los Angeles, CA
[2]Indiana University, Bloomington, IN
[3]West Virginia University, Morgantown, WV
[4]Northern Arizona University, Flagstaff, AZ
[5]University of California, Riverside, Riverside, CA

Contact: jbfisher@jpl.nasa.gov

BER Program: TES
Project: University Award

This MODEX project advances plant-soil-microbial dynamics in terrestrial biosphere/Earth system models in three areas: i) nutrient cycling and plant uptake (nitrogen and phosphorus); ii) root exudation and priming; and, iii) mycorrhizal dynamics. We leverage a 6-site mycorrhizal gradient across the US to develop the Fixation & Uptake of Nitrogen (FUN) submodel, embedded within CLM 5.0. FUN-CLM specifies the site data collection, which includes soil, leaf chemistry, and litterfall sampling from nine plots (3 ectomycorrhizal, ECM; 3 arbuscular mycorrhizal, AM; 3 mixed) at each of the 6 sites. A remote sensing component expands the observational constraints to the model globally.

Initial site-level results show that ECM plots are more nutrient limited than are AM or mixed plots. ECM plots also have lower soil pH, higher soil C:N, and higher lignin:N in leaf litter. Moreover, ECM plots had lower microbial growth efficiency than AM plots, likely reflecting the necessity for greater enzyme investment by ECM soil microbes to degrade soil organic matter; this is supported by higher rates of lignolytic enzymes activity. Long-term monitoring and experiments have begun with the installation of minirhizotron tubes, root ingrowth cores, and ^{13}C isotopically distinct soil cores to monitor net belowground inputs.

Concurrently, we are developing the C cost of P uptake computational framework in FUN, as well as the additional C and N cost of synthesizing phosphatase enzymes to extract P from soil (FUN- P). The model is currently parameterized with the initial site-level data, as well as previous data at a subset of the sites, resulting in differences in costs, uptake, and nutrient cycling between ECM and AM trees in the model. Initial results show that FUN-P accurately estimates empirical measurements of P retranslocation to leaves across the sites. Further, the inclusion of costs for P uptake improves the ability of the model to capture observed patterns in C allocation to root exudation and mycorrhizal biomass. The modeling framework setup will facilitate dynamic ingest of new data as they come online from the empirical work. Collectively, the modeling activity provides a novel framework for understanding how interactions between the C-N-P cycles belowground impact the ability of plants to acquire nutrients and support NPP.

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

Poster #1-30

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

Jennifer Fraterrigo[1,2,3*], Weile Chen[1], Feng Sheng Hu[2,3], Ken Tape[4], and Eugenie Euskirchen[5]

[1]Department of Natural Resources and Environmental Sciences, University of Illinois;
[2]Program in Ecology, Evolution, and Conservation Biology, University of Illinois;
[3]Department of Plant Biology, University of Illinois;
[4]Institute of Northern Engineering, Water and Environmental Research Center, University of Alaska Fairbanks, Fairbanks, AK
[5]Institute of Arctic Biology, University of Alaska Fairbanks, Fairbanks, AK

Contact: jmf@illinois.edu

BER Program: TES
Project: University Award

Arctic plant communities are changing in response to climate 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. We are investigating how above- and belowground plant functional traits respond to environmental conditions and affect belowground carbon stocks and fluxes. In summer 2017, we measured the traits of three shrub species, *Alnus viridis* ssp. *fruticosa*, *Salix richardsonii* and *Betula nana*, in five sites spanning a climate gradient in northern Alaska. Within each site, we collected leaf and root samples from ten individuals per species along a thaw gradient, from riverside to upland, moist tussock tundra. Preliminary findings demonstrate a hierarchy of controls on leaf traits. Regionally, shrub SLA was negatively related to number of growing degree days ($P=0.02$), indicating that investment in leaf construction increases with growing season length, as expected for leaves with a longer life-span. Given that SLA and net photosynthetic rate are positively correlated, our findings suggest that net C assimilation rates of shrubs will decrease with sustained summer warming. Locally, however, shrub SLA varied with active layer thickness, climate zone, and species. In warmer southern sites, we observed a positive relationship between alder SLA and active layer thickness ($P=0.08$), and no relationship for birch or willow. In the cooler northern sites, we observed a positive relationship between SLA and active layer thickness for willow ($P=0.03$), a weak negative relationship for birch ($P=0.09$), and no relationship for alder. We observed a negative relationship between SLA and specific root length (SRL) at the regional scale ($P<0.001$), but patterns of trait covariation differed with climate and by species. In the north sites, we found no evidence that shrub SLA varied with SRL. Covariation between SLA and SRL was stronger in the southern sites, where active layers were deeper. Collectively, our shrub trait data demonstrate that species within the shrub PFT respond differently to environmental variation, resulting in above- and belowground trait distributions that differ considerably across space. This underscores the limitations of using fixed trait values to characterize tundra PFTs. 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 #1-60

Carbon Dynamics Across the Terrestrial-Aquatic Interface of Subtropical Ecosystems in Central Florida

Ross Hinkle[1*], Brian Benscoter[2], Xavier Comas[2], Matthew McCllelan[2], K. Elizabeth Becker[1], and Scott Graham[3]

[1]University of Central Florida, Orlando, Fl;
[2]Florida Atlantic University, Davies, Fl;
[3]Manaaki Whenua Landcare Research, Lincoln, NZ

Contact: rhinkle@ucf.edu

BER Program: TES
Project: University Award

Low-latitude coastal zones are complex landscapes that transition spatially from xeric pine forests on sandy soils to isolated or expansive wetlands with thick hydric soils. These terrestrial- aquatic interfaces have considerable influence on regional-to-global carbon (C) cycles; therefore, representation of these complex, diverse landscapes in Earth System Models (ESMs) is critical. In this project, we use multi-scale C cycle assessments at forest and wetland ecosystems of Disney Wilderness Preserve (DWP) and Blue Cypress Marsh (BCM) in central Florida to evaluate key process and ecosystem characteristics across this hydrologic continuum. Measurements of atmospheric C flux and biomass C stocks have been made in a longleaf pine flatwoods (DWPF) and depression marshes (DWPM) at DWP and a subtropical peatland (BCM), which have captured with multiple prescribed fire events and interannual hydrologic extremes. We found these ecosystems typically serve as a net sink of C; however, the systems become a net source of C immediately following a fire event, recovering to a net sink of C ~6 weeks postfire for herbaceous wetlands (DWPM and BCM) and ~2 months for the pine flatwoods. Using ground penetrating radar approaches, isolated wetlands within the pine flatwoods landscape were shown to be important contributors to the landscape carbon budget. The pine flatwoods site sequestered 190-510 g C m^2 y^{-1}; while ~450 g C m^{-2} was lost during a prescribed fire, the site recovered the biomass C lost from the fire within 2.5 years (the typical fire return interval for this ecosystem is 3 years). At the BCM wetland, hydroperiod was a strong driver of net ecosystem productivity, which was relatively low (65-97 g CO_2-C m^{-2} y^{-1}) in years with periodic drying events (9 mo. hydroperiod) and much greater (284-597 g CO_2-C m^{-2} y^{-1}) during years with constant marsh inundation. Lower rates were primarily the result of increased peat oxidation during periods when marsh water level was below land surface at BCM. Methane emissions from BCM were 38 g CH_4-C M^{-2} y^{-1}, varying seasonally with temperature and water level, while methane emissions from DWPM was 66 g CH_4-C m^{-2} y^{-1}. Simulations of long-term C balance (accounting for drought and fire) indicate the BCM site is a sink for 131 g C m^{-2} y^{-1}. The study found these ecosystems are carbon sinks even in the context of fire and hydrologic disturbances.

Poster #1-54

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

Anya Hopple[1*], Kaitlin Brunik[1], Laurel Pfeifer-Meister[1], Jason K. Keller[2], Glenn Woerndle[2], Cassandra A. Zalman[2], Paul Hanson[3], and Scott D. Bridgham[1*]

[1]Institute of Ecology and Evolution, University of Oregon, Eugene, OR
[2]Schmid College of Science and Technology, Chapman University, Orange, CA
[3]Environmental Sciences Division, Oak Ridge National Lab, Oak Ridge, TN

Contact: ahopple@uoregon.edu

BER Program: TES
Project: University Award

Peatlands are among Earth's most important terrestrial ecosystems due to their massive soil carbon (C) stores and significant release of methane (CH_4) into the atmosphere. Methane has a sustained-flux global warming potential 45-times greater than carbon dioxide (CO_2), and the accuracy of Earth system model projections relies on our mechanistic understanding of peatland CH_4 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 CO_2 and CH_4 production, as well as the anaerobic oxidation of CH_4 (AOM), in a boreal peatland following 13 months of deep peat heating (DPH) and 16 months of subsequent whole-ecosystem warming (surface and deep heating; WEW) as part of the Spruce and Peatland Responses Under Changing Environments (SPRUCE) project in northern Minnesota, USA. The study uses a regression-based experimental design including 5 temperature treatments that warmed the entire 2 m peat profile from 0 to +9°C above ambient temperature. Soil cores were collected at multiple depths (25-200 cm) from each experimental chamber at the SPRUCE site and anaerobically incubated at in situ temperatures for 1-2 weeks. Methane and CO_2 production in surface peat were positively correlated with elevated temperature, but no consistent temperature response was found at depth (75-200 cm) following DPH. However, during WEW, we observed significant increases in both surface and deep peat methanogenesis with increasing temperature. Surface peat had greater CH_4 production rates than deeper peat, implying that the increased CH_4 emissions observed in thefield were largely driven by surface peat warming. The CO_2:CH_4 ratio was inversely correlatedwith temperature across all depths following 16 months of WEW, indicating that the entire peat profile is becoming more methanogenic with warming. We also observed AOM throughout the whole peat profile, with the highest rates observed at the surface and initial data suggesting a positive correlation with increasing temperature. While SPRUCE will continue for many years, our initial results suggest that the vast C stores at depth in peatlands are minimally responsive to warming and any response will be driven largely by surface peat.

Poster #9-37

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

Valeriy Ivanov[1*], Scott R. Saleska[2], Dennis G. Dye[3], Alfredo Huete[4], Neill Prohaska2[2], Loren Albert[2], Rodrigo da Silva[5], Bruce Nelson[6], Luiz Aragao[7], Marciel J. Ferreira[8], Mauro Brum[9], Rafael Oliveira[9], Elizabeth Agee[1], Gabriele Manoli[10], and Simone Fatichi[10]

[1]University of Michigan, Dept. of Civil and Environmental Engineering
[2]University of Arizona, Dept. of Ecology and Evolutionary Biology
[3]Earth Vision Science and Technology Center (formerly at the U.S. Geological Survey, Western Geographic Science Center)
[4]University of Technology, Sydney, Australia
[5]Federal University of West-Para (UFOPa), Santarem, Brazil
[6]National Institute of Amazonian Research (INPA), Brazil
[7]National Institute for Space Research (INPE), Brazil
[8]Federal University of Amazonas (UFAM), Brazil
[9]Institute of Biology, State University of Campinas, Brazil
[10]Institute of Environmental Engineering, ETH Zurich, Zurich, Switzerland.

Contact: ivanov@umich.edu

BER Program: TES
Project: University Award

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 level of hydration. 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. 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 conclude that representation of hydraulic traits is necessary for reliable modeling of the seasonal dynamics of photosynthesis. Tower-based phenology cameras show that synchronization of new leaf growth shifts canopy composition toward younger, more light-use efficient leaves, thus explaining large seasonal increases in ecosystem photosynthesis. We present a new scheme to include such age-dependent variation among individual leaves and crowns into models and incorporate it into state-of-the-art eco-hydrological model Thetys & Chloris (T&C). Using simulations, we assess the impact of leaf phenology on the seasonality of biosphere-atmosphere exchanges in the Amazon across a range of sites, suggesting a new strategy for mapping traits to function of tropical forests in the next generation of predictive models of ecosystem dynamics.

Poster #1-55

Toward the Predictive Understanding of Greenhouse Gas Production in High Latitude Peatlands

Joel Kostka[1*], Max Kolton[1], Rachel Wilson[2], Malak Tfaily[3], Jeff Chanton[2], William Cooper[2], and Chris Schadt[4]

[1]Georgia Institute of Technology, Atlanta, GA
[2]Florida State University, Tallahassee, FL
[3]Pacific Northwest National Laboratory, Richland, WA
[4]Oak Ridge National Laboratory, Oak Ridge, TN

Contact: joel.kostka@biology.gatech.edu

BER Program: TES
Project: University Award

Arctic and boreal peatlands represent critical regions that cover only 3% of the Earth's land surface but store approximately 1/3 of all soil carbon (C), and currently act as atmospheric C sinks. While future warming and CO_2 enrichment should accelerate peat decomposition, uncertainty in the size and reactivity of peat C stocks is cited as a barrier to the reliable predictive modeling of the resilience of belowground C reservoirs to future perturbations and the release of greenhouse gases (GHGs) to the atmosphere. Thus, the goals of this project are to investigate peatland soil organic matter (SOM = peat + dissolved organic matter, DOM) recalcitrance and alternative mechanisms of electron flow as primary controls over belowground C turnover, GHG production (CO_2:CH_4) ratios, and the response of the microbial C cycle to climatic forcing. 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.

We have previously shown (1) that heterotrophic respiration within the peat at SPRUCE is largely driven by DOM and (2) that shallow depths are most susceptible to enhanced warming. Thus any increases in labile organic matter inputs to surface soil, in particular, are likely to result in significant changes to CO_2 and CH_4 production. Multiple field campaigns were conducted in summer 2017 to capture the whole ecosystem response after 2 years of whole- ecosystem warming (WEW). The DOM metabolome and microbial communities were characterized using advanced analytical chemistry techniques and environmental genomics, respectively. Depth remains the greatest driver of variability across the site, reflecting the trend of increasing humification and parallel microbial community stratification with depth. However, we did find significant correlations between metabolite concentrations and temperature treatment for small sugars, amino acids, and some lipids in surface peat (≤50 cm). In general, small sugars and diacylglycerols increase, while amino acid concentrations decrease with temperature. These results are consistent with increased availability of labile substrates promoting increases in microbial biomass that draw down the pool of available free amino acids in the porewater. Further results suggest that plant stress compounds are increasing, likely in response to warmer temperatures and dryer conditions in the treatment plot which may alter the supply of both C substrates and electron acceptors available for heterotrophic respiration.

Because destructive core sampling is limited within the enclosures, our group is exploring the response of porewater microbial communities to WEW. Surprisingly, microbial diversity in porewater was shown to be equal to or higher in comparison to peat. In response to WEW, preliminary results indicate that microbial diversity declined in porewater and microbial communities show a pronounced shift in composition. In particular, an increase in the relative abundance of methanogens and methanotrophs was observed.

Poster #1-61

Coastal Wetland Carbon Sequestration in a Warmer Climate

Pat Megonigal[1*], Genevieve Noyce[1], Roy Rich[1], Matthew Kirwan[2], Ellen Herbert[2], Peter Thornton[4], Teri O'Meara[4], Glenn Guntenspergen[5], Joshua Jones[5], and Paul Dijkstra[3]

[1]Smithsonian Environmental Research Center
[2]Virginia Institute of Marine Sciences
[3]Northern Arizona University
[4]Oak Ridge National Laboratory
[5]US Geologic Survey

Contact: megonigalp@si.edu

BER Program: TES
Project: University Award

Coastal wetlands are global hotspots of carbon storage. The future sink strength and carbon stock stability of these systems is uncertain because global change drivers such as temperature and elevated CO_2 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. The experiment has a gradient design with four aboveground and soil warming treatments ranging from 0 to +5.1^{O}C, to a soil depth of 1.5 m. Elevated CO_2 is crossed with temperature at the treatment extremes (0, +5.1 ^{O}C). Replicate transects (n=3) are located in each of two plant communities that vary in flooding frequency.

C_3 and C_4 communities responded differently to warming. Net primary production (NPP) in the C_3 community increased initially at +1.7°C, but changed little with additional warming. By contrast, NPP in the C_4 community declined monotonically with increasing warming. Different responses may be due to greater heat-related stress in the relatively dry conditions of the C_4 site compared to the C_3 site. Belowground NPP in the C_3 community doubled at +1.7°C, but declined with additional warming. The decline in belowground NPP was entirely compensated by higher aboveground NPP, which drove a decline in the root:shoot ratio. Nitrogen fertilization produces the same pattern in an elevated CO_2 x N study at our site (Langley et al. 2009), suggesting that the decline in root:shoot ratio is a response to a warming-induced rise in N mineralization rates. Plants typically shift growth allocation to aboveground tissue when N limitation is relieved. The C_4 community was generally less responsive to warming, particularly above +1.7^{O}C. Elevated CO_2 increased total NPP at both the +0 ^{O}C and +5.1 ^{O}C treatments, especially belowground NPP at +5.1^{O}C.

CH_4 emissions increased non-linearly with temperature and gross primary production in both plant communities. Elevated CO_2 significantly decreased CH_4 emissions at +0 and +5.1^{O}C, which is likely due to higher root biomass, increased O_2 flux o from roots to the rhizosphere, and stimulation of aerobic CH_4 oxidation.

Our initial results suggest that warming alone will decrease soil C sequestration due to a decline in root production, and increase CH_4 emissions, causing net radiative forcings. However, elevated CO_2 may offset these effects in C_3-dominated plant communities.

Poster #9-38

Variation in the Soil Template Drives Large Variation in Forest Functioning, Composition, and Structure During Tropical Dry Forest Secondary Succession

David Medvigy[1*], Forrest Hoffman[2], Xiaojuan Yang[2], Bonnie Waring[3], Annette Trierweiler[1], German Vargas[4], Camila Pizano[5], Beatriz Salgado[6], Juan Dupuy[7], Catherine Hulshof[8], Gangsheng Wang[2], Qing Zhu[9], Skip Van Bloem[10] and Jennifer Powers[4]

[1]Notre Dame University, South Bend, IN
[2]Oak Ridge National Laboratory, Oak Ridge, TN
[3]Utah State University, Logan, UT
[4]University of Minnesota, St. Paul, MN
[5]ICESI University, Cali, Colombia
[6]Universidad del Norte, Baranquilla, Colombia
[7]Yucatán Center for Science Investigation (CICY), Merida, Yucatán, Mexico
[8]Virginia Commonwealth University, Richmond, VA
[9]Lawrence Berkeley National Lab
[10]Clemson University, Clemson, SC

Contact: dmedvigy@nd.edu

BER Program: TES
Project: University Award

Observations of tropical forests have revealed large variations in aboveground biomass, plant composition, ecosystem structure, and biogeochemical functioning across plots. A relatively large amount of variability remains even when precipitation and stand age are controlled for. Here, we analyze the extent to which variability in ecosystem processes and characteristics can emerge from solely from variation in the soil template. We performed controlled experiments using a mechanistic, numerical model. The model dynamically couples ED2 (vegetation dynamics), MEND (biogeochemistry), and N-COM (plant-microbe competition for nutrients). Here, the MEND-component of the model has been extended to include nitrogen and phosphorus cycles. We focus on simulation of eighteen 0.1-hectare forest inventory plots in Guanacaste, Costa Rica that were established in 2008. All plots experience statistically similar climate conditions, but vary greatly in terms of soil texture, soil percent carbon (C), carbon-to-nitrogen (N) ratios, extractable phosphorus (P), total P, and other soil properties. We predicted that our simulations would show that (1) ecosystem-level state variables would vary between the plots because of differences in nutrient limitation, (2) because of non-linearities in nutrient cycling, a single simulation forced with average soil conditions would differ from the average of the eighteen simulations that resolved variability in the soils, (3) because different plant functional types (PFTs) have different nutrient requirements, variation in the soil template would lead to variation in PFT composition.

These three predictions were confirmed by model simulations. After 40 years of secondary succession, the spread in plant biomass was about 40% of the mean. The accumulated biomass was positively correlated with the initial amount of non-occluded soil P. Ecosystem structure also varied, with the height of the centroid of leaf area index (LAI) also being correlated to non-occluded soil P. A simulation with artificially large N and P deposition rates had a much smaller spread in accumulated aboveground biomass, confirming a nutrient limitation dynamic. The proportional amounts of different PFTs simulated in the different plots also varied widely and depended on differing degrees and N and P limitation. Overall, our simulations provide a mechanistic link between realistic variations in the soil template and large variation in ecosystem functioning, composition, and structure during secondary succession. Because of these strong linkages between the soil template and emergent ecosystem

characteristics, we suggest that the grid structure of regional and global models better account for variations in the soils.

Poster #9-39

Extrapolating Ecosystem Processes of Seasonally Dry Tropical Forests Across Geographic Scales and into Future Climates

Jennifer Powers[1*], David Medvigy[2], Forrest Hoffman[3], Xiaojuan Yang[3], Bonnie Waring[4], Annette Trierweiler[2], German Vargas[1], Camila Pizano[5], Beatriz Salgado[5], Juan Dupuy[6], Catherine Hulshof[7], and Skip Van Bloem[8]

[1]University of Minnesota, St. Paul, MN
[2]Notre Dame University, South Bend, IN
[3]Oak Ridge National Laboratory, Oak Ridge, TN
[4]Utah State University, Logan, UT
[5]ICESI University, Cali, Colombia
[6]Yucatán Center for Science Investigation (CICY), Merida, Yucatán, Mexico
[7]Virginia Commonwealth University, Richmond, VA
[8]Clemson University, Clemson, SC

Contact: powers@umn.edu

BER Program: TES
Project: University Award

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. It is unknown whether SDTFs are uniquely vulnerable or resilient to global environmental changes including climate change and increasing drought[1]. We hypothesize that the responses of STDFs to global change depend critically on belowground processes and nutrient availability, but we lack empirical data to verify this. Our objectives are to quantify how above- and belowground processes mediate the responses of SDTF carbon dynamics to environmental change, and to 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 and hydraulic 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. Our empirical studies are yielding interesting results. First, results from our nitrogen and phosphorus addition experiment show rapid responses of plant symbionts to nutrient addition: legume nodule production increased in plots fertilized by P, but not N+P or N alone, and root colonization by arbuscular mycorrhizal fungi decreased in the N+P treatment only. Plant species displayed a range of stem growth responses to factorial N and P fertilization. Second, we established a large-scale 50% throughfall exclusion experiment that is crossed with a complete nutrient fertilization treatment. Stem growth of the six focal species responded individualistically to the treatments. Many species showed reductions in stem growth with drought; however, in several species fertilization modulated the responses to drought. Five out of six species showed increased growth in the fertilization treatment. Collectively these studies suggest that nutrient availability is an important constraint on tropical dry forest ecosystem processes and responses to rainfall reduction. Our third project provides detailed data on how soil biogeochemistry and forest growth varies across the range of Neotropical dry forests. These data suggest enormous variation in the structure and ecosystem processes among forests and serve as the basis for modeling.

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Poster #9-5

Improving our Understanding, Quantification, and Contextualization of Dryland Feedbacks to Climate Change

Sasha Reed[1], Colin Tucker[1], Scott Ferrenberg[2], Tim Wertin[3], Armin Howell[1], Robin Reibold[1], Austin Rutherford[4], and Jayne Belnap[1]

[1] Southwest Biological Science Center, Moab, UT
[2] New Mexico State University, Las Cruces, NM
[3] University of Illinois, Urbana-Champaign, Champaign, IL
[4] University of Arizona, Tucson, AZ

Contact: screed@usgs.gov

BER Program: TES
Project: University Award

Due to their large spatial extent and high responsiveness to climate variability, 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 interact to affect dryland feedbacks to climate remains notably poor. In particular, while the data we do have suggest a strong potential for drylands to cross climate thresholds and for climate-induced changes in drylands to create large feedbacks to future climate, we need significant improvement in our quantification of dryland feedbacks, as well as 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 drylands on the Colorado Plateau, USA. Using automated CO_2 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 CO_2 between the atmosphere and dryland soils (including biological soil crusts) that is strongly controlled by surface (0-2 mm) soil climate conditions, which would be incorrectly estimated using deeper traditional soil sensors. Our data show how biocrust CO_2 fluxes are partitioned into net primary productivity and respiration, how these discrete fluxes are differentially affected by climate, and how they are quantitatively and temporally related to CO_2 exchange for the site's vascular plants. The data also show the strong role of biocrust community composition in affecting ecosystem energy balance. Taken together, these data represent a step forward in our understanding of and capacity to forecast how dryland organisms, coupled biogeochemical cycles, and energy fluxes will respond to a range of future climates across a diverse biome.

Poster #1-56

Plant–microbe Symbioses Preserve Carbon in Peatlands Along a Latitudinal Gradient from Minnesota to Peru

Curtis J. Richardson[1], Hongjun Wang[1], Suzanne Hodgkins[2], Neal Flanagan[1], Bill Cooper[2], Tian Jianqing[1], Mengchi Ho[1], and Jeff Chanton[3]

[1]Duke University Wetland Ctr., Nicholas School of the Environment, Durham, NC
[2]Department of Chemistry & Biogeochemistry, FSU, Tallahassee, FL
[3]Department of Earth, Ocean and Atmospheric Science, FSU, Tallahassee, FL

Contact: curtr@duke.edu

BER Program: TES
Project: University Award

Peatlands store one-third of soil C in terrestrial ecosystems and have persisted through changing climate over millennia from the arctic to the tropics. Approximately one-third of peat stores are found in subtropical and tropical peatlands (STPs) formed from high-lignin woody biomass. In this project, our questions are: 1) why do these non-*sphagnum* peatlands (STPs) accumulate C under warmer-drier climates and 2) how might insights coming from studying control mechanisms in STPs improve the management and conservation of the vast C stores in boreal peatlands subject to increasing climate forcing. We hypothesized that a dual control or "latch mechanism" reduces decomposition in shrub/tree communities in STPs due to both (1) higher production of polyphenol and aromatic compounds in STPs than found in northern *Sphagnum*/Carex communities and (2) the buildup of recalcitrant organic matter produced by light fire-drought-warming-adapted communities, together leading to a reduction in the microbial decay rate of peat. After three-years of intensive biological and chemical analysis in a series of field and microcosm experiments along our north to south bog gradient from Minnesota to Peru, we show how previously unrecognized biotic factors, particularly dynamic interlinked above- and belowground attributes control C sequestration in peatlands. Our key findings include (1) phenolics-bridged plant-microbe symbioses, principally slow-growing microbes dominated in higher phenolic wooded STPs, preserving C in peatlands under climate change, 2) phenolics are the overarching factor controlling the relative abundance of slow-and fast-growing microbes, the slow-growing microbes in STPs metabolize C slowly and are inherently resistant to disturbance, 3) global data analysis shows that soil respiration does not increase exponentially from boreal to tropical peatlands, suggesting that slow-growing microbes may have become dominant in most non-boreal peatlands, 4) peat chemistry analysis from over 2000 samples show that across peatlands both from the arctic to tropics and from high to low elevation peatlands recalcitrance increases as aromatic content increases, and 5) peat affected by low-severity wildfires displays a similar pattern of higher aromatic content. Our findings all demonstrate links between peat recalcitrance and increased content of phenolics and other aromatic compounds in plants. Thus, linked plant–microbe symbiotic traits are a key to understanding ecological resilience and resistance developed in peatlands under disturbance. New trait-based approaches that can better link above-and below ground processes are needed to advance both the accuracy and precision of current abiotic-factor-based Earth system models in predicting future soil C responses to climate-change feedbacks.

Poster #1-31

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

Edward A. G. Schuur[1*], Rosvel Bracho[2], Gerardo Celis[1], Kathryn G. Crummer[2], Chris Ebert[1], Jack Hutchings[3], Caitlin Pries[4], Marguerite Mauritz[1], Elaine Pegoraro[1], César Plaza[1], Susan Natali[5], Verity Salmon[6], Christina Schaedel[1], Meghan Taylor[1], Elizabeth Webb, Charlie Koven[7], and Yiqi Luo[1].

[1]Center for Ecosystem Science and Society, Northern Arizona University, Flagstaff, AZ
[2] School of Forest Resources and Conservation, University of Florida, Gainesville, FL
[3]Department of Geology, University of Florida, Gainesville, FL
[4]Dartmouth College, Hanover, NH
[5]Woods Hole Research Center, Falmouth, MA
[6]Environmental Sciences Division, Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[7]Climate Sciences Department, Climate and Ecosystem Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: ted.schuur@nau.edu

BER Program: TES
Project: University Award
Project Website: http://www2.nau.edu/schuurlab-p/CiPEHR.html

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. Understanding the magnitude, rate, and form of greenhouse gas release to the atmosphere is crucial for predicting the strength and timing of this carbon cycle feedback to a warming climate. Here we report results from an ecosystem warming manipulation where we increased air and soil temperature, and degraded the surface permafrost. We used snow fences coupled with spring snow removal to increase deep soil temperatures and thaw depth (soil warming) and open top chambers to increase growing season air temperatures (air warming). The soil warming treatment has successfully warmed soils by 2-3ºC in winter, has increased growing-season depth of ground thaw by up to 50%, and has degraded an increasing amount of surface permafrost each year of the project. We have subsequently manipulated the surface water table that together with warming influences air and deep soil temperatures, permafrost, and soil moisture conditions that are primary drivers of tundra ecosystem carbon balance across the Arctic landscape. Here we report measurements of long-term carbon dioxide and methane exchange as a metric of changes in ecosystem carbon storage. Overall, soil warming had a much stronger effect on carbon exchange than air warming, and the dynamics changed non-linearly over the course of the long- term experiment. Soil warming that degraded permafrost stimulated both gross primary productivity (GPP) and ecosystem respiration (ER) such that the system was initially a net sink of C in the growing season over the first five years of the experiment. In the second phase (6-9 years), ground subsidence as a result of thaw continued to increase soil moisture and saturate the soil. While permafrost thaw as a result of the manipulation continued to progress in these years, both GPP and ER became suppressed and resulted initially in neutral growing season C exchange, and eventually net C release (source). Soil warming has altered not only the rates of C exchange but also the form of C, as measurements have now documented an increase in CH_4emissions where soils are wetter as a result of permafrost degradation. Increased flux in combination with the higher global warming potential of CH_4 contributes to the overall climate impact of permafrost thaw. This dynamic is likely to change in the future as the permafrost table is driven deeper into the ground.

Poster #9-35

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

Christine S. O'Connell[1] and Whendee L. Silver[1*]

[1]University of California, Berkeley, Berkeley, California

Contact: coconn@berkeley.edu

BER Program: TES
Project: University Award

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 (O_2) 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 (CO_2), nitrous oxide (N_2O), and methane (CH_4). 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. We found that 5%, 3% and 7% of CO_2, N_2O and CH_4 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 CO_2 by 25% (from 2.16 to 2.69 umol/m2/s), the mean flux of N_2O by 10% (from 0.10 to 0.11 nmol/m2/s), and the mean flux of CH_4 by 77% (from 2.07 to 3.66 nmol/m2/s). Soil moisture and O_2 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 O_2 concentrations also experienced oscillations over hours, days and months. Soil O_2 concentrations were correlated positively with CO_2 fluxes (pearson's coefficient = 0.25) and negatively with N_2O and CH_4 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 #1-68

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

Carl Trettin[1*], Andrew Burton[2], Martin Jurgensen[2], Zhaohua Dai[2]. Brian Forschler[3], Jonathan Schilling[4]. Debbie Page-Dumroese[1], and Daniel Lindner[1]

[1]USDA Forest Service
[2]Michigan Technological University
[3]University of Georgia
[4]University of Minnesota

Contact: ctrettin@fs.fed.us

BER Program: TES
Project: University Award

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

The FACE Wood Decomposition Experiment (FWDE) was established with wood grown under the elevated CO_2 in the free-air carbon dioxide enrichment (FACE) experiment. By using that $\delta^{13}C$ signature in three species of wood from two FACE sites, we are effectively continuing the FACE experiment by using wood grown under elevated CO_2 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 is being conducted principally on the continental-scale (FWDE), where ambient and elevated CO_2 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. Assays from the FWDE affirm that the $\delta^{13}C$ signature of the FACE wood can be traced into the mineral soil. A field campaign was completed in 2017 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. Also, during 2017, the framework for a module within Forest DNDC was developed 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.

Terrestrial Ecosystem Science

Next Generation Ecosystem Experiments (NGEE): Arctic

Poster #1-6

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

Stan Wullschleger[1*], Tom Boden[1], Robert Bolton[5], David Graham[1], Susan Hubbard[3], Colleen Iversen[1], Alistair Rogers[4], Vladimir Romanovsky[5], Joel Rowland[2], Peter Thornton[1], Margaret Torn[3], William Riley[3], and Cathy Wilson[2]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Los Alamos National Laboratory, Los Alamos, NM
[3]Lawrence Berkeley National Laboratory, Berkeley, CA
[4]Brookhaven National Laboratory, Upton, NY
[5]University of Alaska, Fairbanks, AK

Contact: wullschlegsd@ornl.gov

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

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 Utqiaġvik) 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 Energy Exascale Earth System Model (E3SM). 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 CO_2 and CH_4 fluxes across a range of permafrost conditions, (3) variation in plant functional traits across space and time, and in response to changing environmental conditions, (4) controls on shrub distribution and associated climate biogeochemical and biophysical feedbacks to climate, and (5) changes in surface and groundwater hydrology. Our vision 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 #1-7

Coupling PFLOTRAN into E3SM through a Collaboration between the CMDV and NGEE Arctic Projects

Gangsheng Wang[1*], Fengming Yuan[1], and Peter Thornton[1]

[1]Environmental Sciences Division, Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: wangg@ornl.gov

BER Program: CMDV
Project: CMDV and NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

Microbially-explicit soil biogeochemistry (BGC) models are thought to be more biologically realistic than conventional models, and improved model structures can potentially better represent field- and lab-scale observations. 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 interface in the Energy Exascale Earth System Model (E3SM) through the CMDV project. The interface facilitates the coupling of PLFOTRAN into the E3SM Land Model (ELM). The development of this interface is to enable flexible and fast development and evaluation of soil BGC modules and their coupling to various thermal- hydrology (TH) and aboveground vegetation modules. The interface includes a generic data- structure to pass data between submodels (i.e., vegetation, TH and BGC) and allows users to select a specific submodel from multiple options (e.g., ELM-BGC or PFLOTRAN-BGC for BGC). We evaluate ELM-PFLOTRAN and compare it to the original ELM and observations at a field site near Barrow (recently renamed Utqiaġvik), AK. The ELM-PFLOTRAN simulations (e.g., GPP, LAI, and total soil organic carbon) were improved by modifying the nitrogen (N) uptake profile with N fixation profile (representing root distribution). Without this improvement, there is not enough N in ELM-PFLOTRAN to support plant growth and accumulation of SOM during model spin-up. Further coupling of PFLOTRAN-TH into ELM is underway and the coupled PFLOTRAN TH-BGC will be tested at both point and regional scales.

Poster #1-8

Remote Sensing of the Spatial and Temporal Patterns of Arctic Plant Traits and Ecosystem Function

Shawn Serbin[1*], Ran Meng[1], Andrew McMahon[1], Wil Lieberman-Cribbin[1], Kim Ely[1], Alistair Rogers[1], and Stan Wullschleger[2]

[1]Brookhaven National Laboratory
[2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: sserbin@bnl.gov

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

The inadequate representation of plant trait variation across space and time in terrestrial biosphere models, including many that underlie the land-surface component of Earth System Models, is a key uncertainty in model projections of terrestrial carbon, water, and energy fluxes and storage. This is particularly relevant for biomes with historically sparse observational data, such as high latitudes of the Arctic where uncertainty in the modeling of carbon uptake and associated processes has been attributed to plant properties that regulate these processes. An approach is needed to bridge the scales between detailed ongoing *in-situ* 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 data, particularly spectroscopy and imaging spectroscopy (IS), high resolution imaging, and thermal infrared (TIR) thermography, represent important observational datasets capable of scaling plant properties and capturing broad-scale spatial and temporal dynamics in many important vegetation properties, offering an important and direct data constraint on model projections or as critical benchmarks against prognostic model predictions. Here we extend the approaches developed for temperate ecosystems to derive scaling algorithms for a broad range of plant traits across the high Arctic, including biochemical, morphological and physiological leaf traits from the leaf to landscape scales. We focus on the linkages between a range of plant species and remote sensing data within our core study areas within the Barrow Environmental Observatory (BEO), Barrow (recently renamed Utqiaġvik), and Nome Alaska regions. 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), TIR, and optical imagery from near-surface (leaf, tram) to unmanned aerial system (UAS) platforms. We show how leaf-level spectra-trait models for Arctic vegetation, developed using data collected in the BEO during the 2014-2017 growing seasons, are comparable with existing models from other biomes. In addition, tram and UAS platforms show a strong capacity to scale traits to the larger landscape and capture patterns through time. We then tested the capacity to map traits by leveraging IS data collected at the Council study site as part of the NASA ABoVE airborne campaign. Our preliminary analyses indicate that our existing approaches can be used with ABoVE imagery to map traits across larger region and provide maps of key traits across the Arctic.

Poster #1-9

Characterization of Permafrost Landscapes Using an Unmanned Aerial System: LiDAR Mapping the NGEE Teller Site

Christian Andresen[1*], Adam Collins[1], Erika Swanson[1], Lauren Charsley-Groffman[1], and Emily Schultz-Fellenz[1], and Cathy Wilson[1]

[1]Los Alamos National Laboratory, Los Alamos, NM

Contact: candresen@lanl.gov

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

We surveyed the NGEE Arctic Teller research site (~3km^2) in August 2017 with an Unmanned Aerial System (UAS). A state-of-the-art Light detection and Ranging (LiDAR) scanner onboard the UAS acquired centimeter-resolution topography data in the form of a point-cloud. In addition to LiDAR, the UAS was equipped with a digital camera that collected high-resolution aerial imagery at 24 Megapixels. Preliminary Lidar and Photogrammetry datasets and associated derived products are presented here. The LiDAR point cloud datasets have a density of 740 points/m^2 and a DEM resolution of 2cm. The LiDAR point-cloud of Teller site will serve as a keystone dataset to better understand the association and co-dependence between topography and multiple environmental processes related to hydrology, geochemistry, geomorphology as well as the relationship between ecosystem structure and function.

Poster #1-10

Complexity of CO_2, CH_4 and Energy Exchange Measurements at NGEE Arctic Sites, Alaska

Sigrid Dengel[1*], Ori Chafe[1], Margaret Torn[1], and Stan Wullschleger[2]

[1]Climate Sciences, Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: sdengel@lbl.gov

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

Two sites with continuous permafrost were established as part of Next-Generation Ecosystem Experiments (NGEE Arctic) to measure ecosystem scale gas exchange via Eddy Covariance (EC): Utqiaġvik (Barrow - US-NGB, Arctic coastal plain polygon tundra) in 2012 and Council (US-NGC), a subarctic lichen rich tussock tundra in 2017. Both sites (also registered AmeriFlux sites) have ongoing CO_2, CH_4, and energy exchange measurements. In order to measure these exchanges we are applying the EC method, a micrometeorological technique. The atmosphere contains turbulent motions of upward and downward moving air that transport trace gases. The EC method provides the measurement of this vertical flux of transported air parcels by correlation of the fluctuations in CO_2 or CH_4 with fluctuations in vertical wind speed. Measurements at US-NGB show a high degree of inter-annual and seasonal variability in meteorology and fluxes. This site encounters a very short complete snow-free season of approximately two months despite a several months long Polar day. Despite being established only July 2017, US-NGC also shows distinctive flux distributions, enabling first impressions of the heterogeneity of this tussock tundra environment. In order to interpret this variability and decipher these diverse fluxes, we apply a variety of models, such as footprint analyses and light response models. In the High Arctic, these data analyses and interpretations come with challenges not experienced in lower latitudes. For example, nighttime definition and data partitioning is critical for accurately estimating respiration rates; however, Arctic sites experience 24 h daylight during summer months (Polar day), making it difficult to partition between day and night. Respiration estimates are required to determine the gross primary productivity of an ecosystem and its ability and efficiency in converting light into photosynthate and thus carbon. Additionally, the quality (UV light) and quantity (longer path length) of light received at high Arctic sites differs significantly from lower latitudes. Furthermore, these sites have several weeks without rising sun over the winter months (Polar night), causing hoar frost to accumulate on transducers and exposed mirrors of EC instruments. The frost creates large gaps in data collection, making year-round measurements in high latitudes challenging; in lower latitudes, the rising sun melts the frost, causing only a few hours of gaps rather than continuous gaps. Continuous CO_2, CH_4, and energy eddy flux measurements at NGEE Arctic sites improves our understanding of these ecosystems, which can be implemented into earth system models and improve the fidelity of model predictions.

Poster #1-11

Multiscale Data Integration for Scaling Land-atmosphere Carbon Exchange and Soil Properties in Ice-wedge Polygon Tundra

Haruko M. Wainwright[1*] Baptiste Dafflon[1], Rusen Oktem[1], Sigrid Dengel[1], John B. Curtis[1], Margaret S. Torn[1], Jessica Cherry[2], Florian Soom[1], Craig Ulrich[1], Timothy Kneafsey[1], Yuxin Wu[1], and Susan S. Hubbard[1]

[1]Earth and Environmental Sciences, Lawrence Berkeley National Laboratory, Berkeley, CA
[2]NOAA National Weather Service, Alaska-Pacific River Forecast Center, Anchorage, AK

Contact: hmwainwright@lbl.gov

Program: TES
Project: NGEE Arctic
Project Website: http://ngee-arctic.ornl.gov/

This study presents approaches to upscale land-atmosphere carbon exchange and key soil properties from point measurements to the field scale. We developed new methods to estimate net ecosystem exchange (NEE) and soil properties in high resolution (0.5 m by 0.5 m) over the ice-wedge polygon tundra using laboratory through field-based soil analysis, tram and flux tower measurements. We demonstrate our approach at the NGEE Arctic site near Barrow (recently renamed Utqiaġvik), AK. Understanding the spatial distribution of soil properties is critical for predicting future ecosystem behavior. We measured organic matter content, bulk density and ice content from a limited number of cores and also performed nondestructive X-ray computed tomography (CT) scans along the entire length of numerous cores. We trained a neural network algorithm and used it to estimate the fraction of soil constituents along these CT-scans. The classified map of geomorphological features is then used to estimate the distribution of soil characteristics at the landscape scale (750m by 750m). Comparison with ground-based geophysical imagery shows consistent large-scale variation in ice content over the site. The use of CT scans and neural network estimation approaches was shown to be a valuable method for bridging the spatial gap between laboratory and geophysical and remote sensing measurements to provide soil composition information over field relevant scales. A key goal of the NGEE Arctic project is to develop and document approaches for scaling fluxes through considering 'local' scale measurements (such as those obtained from cores or in-situ point field measurements) and larger scales (such as those measured by airborne sensors). We developed a Kalman filter method to explore the scaling of measurements and associated NEE at the site. To do this, we integrated multi-scale, multi-type datasets (including those collected from an automated mobile sensor system, or tram system), as well as airborne lidar and imagery. The tram system provided high-frequency measurements of normalized difference vegetation index (NDVI) along a 68-meter transect, capturing spatial heterogeneity associated with microtopography. We take advantage of the significant correlations between NDVI and NEE from the chamber measurements sparse in time and space. We find that data correlations were most informative when the spatial heterogeneity of NDVI and NEE is high in the peak season, which enabled successful estimation. The results of the NEE estimation using the multi-scale data were compared to the flux tower data by averaging the flux within the tower footprint.

Poster #1-12

Mapping Arctic Representativeness and Vegetation using Data Mining and Machine Learning Techniques

Forrest Hoffman[1*], Jitendra Kumar[1], and Zachary L. Langford[2]

[1]Oak Ridge National Laboratory, Oak Ridge, TN
[2]University of Tennessee, Knoxville, TN

Contact: hoffmanfm@ornl.gov

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

Understanding and modeling the evolution of ecosystem processes and land-atmosphere interactions across heterogeneous landscapes in the Arctic requires accurate characterization of vegetation and soil properties at appropriate spatial and temporal scales. However, resource and logistical constraints limit the frequency and extent of environmental observations, particularly in the Arctic, necessitating the use of high-resolution remote sensing imagery and the development of a systematic sampling strategy to maximize coverage and objectively represent environmental variability at desired scales. We have developed and applied data mining and machine learning methods for stratifying sampling domains, informing site selection, determining the representativeness of measurement sites and networks, and mapping vegetation from sparse samples and from multi-sensor remote sensing fusion. In the first study, multivariate spatiotemporal clustering was applied to down-scaled general circulation model results and data for the State of Alaska to define multiple sets of bioclimatic ecoregions across two decadal time periods. Maps of ecoregions for the present (2000-2009) and future (2090-2099) were produced, showing how combinations of 37 bioclimatic characteristics are distributed and how they may shift in the future. Representative sampling locations were identified on present and future ecoregion maps, a representativeness metric was developed, and representativeness maps for eight candidate sampling locations were produced to inform future site selection. In the second study, we applied data mining to scale up sparse vegetation samples by using multi-spectral remote sensing, and we demonstrated that including phenological information significantly improves the quality of vegetation type predictions. In a third study, we applied a convolutional neural network (CNN) approach to map Arctic vegetation distributions for the Kougarok area on the Seward Peninsula by fusing data from multiple sensors. We tested both supervised and unsupervised classification techniques over a 344 sq km area to generate vegetation classifications at 5 m and 12.5 m resolutions. We subsequently compared two CNN approaches to predict vegetation classes for every pixel within the study area in comparison with an existing vegetation classification map. In a fourth, ongoing study, we combined a digital elevation model and other data to stratify sampling domains across the entire Arctic region. We calculated pan- Arctic representativeness based on a suite of sampling locations operated by international research institutes. This presentation will highlight all of these research applications of large- scale data analytics methods and demonstrate their utility for coordinated measurement and modeling activities in the Next Generation Ecosystem Experiments (NGEE) in the Arctic.

Poster #1-13

Quantifying the Interactions between Soil Thermal and Physical Characteristics, Hydro- geomorphological Conditions and Vegetation Distribution in an Arctic Watershed

Baptiste Dafflon[1*], Emmanuel Léger[1], John Peterson[1], Craig Ulrich[1], Sébastien Biraud[1], Anh Phuong Tran[1], Bhavna Arora[1], Haruko Wainwright[1], Vladimir Romanovsky[2], and Susan Hubbard[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]University of Alaska Fairbanks, Fairbanks, AK

Contact: bdafflon@lbl.gov

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

Improving understanding of Arctic ecosystem functioning and parameterization of process-rich hydro-biogeochemical models require advances in quantifying ecosystem properties, from the bedrock to the top of the canopy. In Arctic regions having significant subsurface heterogeneity, understanding the link between soil physical properties (incl. fraction of soil constituents, bedrock depth, permafrost characteristics), thermal behavior, hydrological conditions and landscape properties is particularly challenging yet is critical for predicting the storage and flux of carbon in a changing climate. This study takes place in Seward Peninsula Watersheds near Nome AK and Council AK, which are characterized by an elevation gradient, shallow bedrock, and discontinuous permafrost. We use a variety of ground-based and aerial measurements together to identify the various subsurface hydro-thermal behaviors in the watershed and to evaluate the multi-dimensional relationships between subsurface and surface properties. To characterize permafrost distribution where the top of permafrost cannot be easily identified with a tile probe (due to rocky soil and/or large thaw layer thickness), we developed a novel technique using vertically resolved thermistor probes to directly sense the temperature regime at multiple depths and locations. These measurements complement electrical imaging, seismic refraction and point-scale data for identification of the various thermal behavior and soil characteristics. Also, we evaluate linkages between the soil physical-thermal properties and the surface properties (hydrological conditions, geomorphic characteristics and vegetation distribution) using UAV- based aerial imaging. Data integration and analysis is supported by numerical approaches that simulate hydrological and thermal processes. Overall, this study enables the identification of watershed structure and the links between various subsurface and landscape properties in representative Arctic watersheds. Results show very distinct trends in vertically resolved soil temperature profiles and strong lateral variations over tens of meters that are linked to zones with various hydrological conditions, including the presence of preferential flow paths in the subsurface. The results also show the presence of several meter thick supra-permafrost zones whit presence of unfrozen water year-round. Finally, significant spatial co-variability exists between permafrost characteristics, vegetation, and geomorphology with graminoid covered area corresponding to zones with most shallow permafrost. The interaction between the various compartments is of strong interest to understand the evolution of the landscape and the permafrost distribution. The obtained information is expected to be useful for improving predictions of Arctic ecosystem feedbacks to climate.

Poster #1-14

Factors Affecting the Spatial Pattern of Snow Distribution at the NGEE Arctic Teller and Kougarok Watersheds

Min Chen[1], Cathy Wilson[1*], Lauren Charsley-Groffman[1], Julian Dann[1], W. Robert Bolton[2], Robert Busey[2], and Stan Wullscheger[3]

[1]Los Alamos National Laboratory, Los Alamos, NM
[2]University of Alaska, Fairbanks, AK
[3]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: cjw@lanl.gov

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

Snow cover plays an important role in the climate, hydrology and ecological systems of the Arctic due to its influence on the water balance, thermal regimes, vegetation and carbon flux. However, the spatial distribution of snow depth and density are poorly represented for arctic regions where high-resolution snow data is limited. Researchers with the DOE Office of Science Next Generation Ecosystem Experiment, NGEE Arctic project, are collecting end of winter snow distribution data at high spatial resolution, and developing approaches to more accurately represent event-based snow redistribution processes. These new approaches are being tailored for application in catchment to regional scale models in order to assess the role of snow spatial variability as it interacts with permafrost hydrology and ecosystem function. We use data from two small catchments in the southern Seward Peninsula to identify key factors that control snow distribution and quantify the relative impacts of those factors. At the NGEE Arctic Teller study area, intensive snow depth surveys (1 to 10 meters scale) were conducted in 2016, 2017 and 2018. These data are being co-analyzed with 2018 survey data from the NGEE Arctic Kougarok study area. In 2017, snow density was measured at about 60 selected intensive snow sampling sites, about 200 meters apart across the Teller study area. The snow water equivalent (SWE) calculated from snow depth and snow density, are correlated with vegetation factors, spatial locations, wind factor and topographic factors at different spatial scales to identify the key factors impacting the spatial distribution of snow. A linear mixed model of fixed and random effects is used to quantify the impacts of different external factors on snow distribution and to describe the spatial autocorrelation of snow distribution. Initial results from the Teller data show that snow spatial distribution was similar between 2016 and 2017; SWE has stronger correlation with the impacting factors than the snow depth; there is strong spatial autocorrelation in SWE distribution at two distinct scales, 16.6 m and 154.5m. SWE distribution was significantly impacted by the following factors in the order of importance: vegetation distribution, micro- topography, macro-topography, sun radiation and wind factor. We expect that our empirical statistical model for end of winter SWE will be used to inform an event-based snow redistribution model for the two study watersheds, and to ultimately estimate seasonally dynamic snow coverage and properties for the Seward Peninsula and pan-Arctic regions.

Poster #1-15

Symbiotic N-fixation by Alder Impacts Nitrogen Availability on a Landscape Scale

Verity G. Salmon[1*], Colleen Iversen[1], Amy Breen[2], Peter Thornton[1], and Stan D. Wullschleger[1]

[1]Environmental Sciences Division, Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]International Arctic Research Center, University of Alaska, Fairbanks, AK

Contact: salmonvg@ornl.gov

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

Alnus viridis subspp. *fruticosa* (alder) is a deciduous shrub that forms a symbiotic relationship with *Frankia* bacteria. These bacteria fix atmospheric nitrogen (N) into biologically available forms within nodules formed on the shrub's roots. Nitrogen is the primary limiting nutrient for Arctic plant productivity so inputs of available N via symbiotic fixation has the potential to alter plant, soil and microbial interactions in these rapidly warming ecosystems. To assess plant available N on a Kougarok hillslope on the Seward Peninsula, AK, we established vegetation plots across six plant communities in 2016. Aboveground biomass, inorganic N and P availability in surface soils, and foliar %N and $\delta^{15}N$ were measured across these six plant communities. Although there was a high degree of variation in observed characteristics across the six plant communities, soil inorganic N availability and foliar %N were highest within plots located near alder shrublands, suggesting that symbiotic N fixation inputs from alder shrublands impacts N availability of neighboring microsites. To quantify N inputs associated with alder at the Kougarok site, in 2017 we measured N fixation rates and nodule biomass associated with tall stature alder individuals (>1.5 m) growing in dense shrublands. Nodule biomass associated with short stature alder (<1.5 m) growing in water tracks across tussock tundra was also assessed. Nodule biomass of Alder growing in shrublands was significantly higher than that of alder growing in water tracks (18.54 g/m^2 vs 3.64 g/ m^2, p =0.03). Inputs of N via symbiotic N fixation were to be driven by nodule biomass rather than rates of N fixation within root nodules. Nodule biomass was therefore compared to aboveground biomass, foliar chemistry, specific leaf area, shrub height, and basal area to identify appropriate scaling metrics. Overall, our results suggest that the inclusion of a N fixing shrub plant function type (PFT) in earth system models would improve the ability of these models to capture nutrient dynamics in Arctic ecosystems.

Poster #1-16

Controls and Rates of Change of Shrub Cover in the Arctic: How do Arctic Dynamic Vegetation Models Differ in Their Results for Future Scenarios?

Amy Breen[1*], Margaret Torn[2], Howard Epstein[3], Eugenie Euskirchen[1], Colleen Iversen[4], Isla Myers-Smith[5], William Riley[2], Verity Salmon[4], Zelalem Mekonnen[2], and Stan D. Wullschleger[4]

[1]University of Alaska, Fairbanks, AK
[2]Lawrence Berkeley National Laboratory, Berkeley, CA
[3]University of Virginia, Charlottesville, VA
[4]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[5]University of Edinburgh, Edinburgh, Scotland

Contact: albreen@alaska.edu

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

Contemporary observations in the Arctic show increased shrub growth and colonization with regional warming and both observations and models suggest that as global climate warms, shrubs will become more widespread pan-Arctic. Compared to low-statured tundra vegetation, shrubs – particularly tall shrubs such as alder, birch and willow – have strong effects on climate through both biophysical and biogeochemical processes, including differences in albedo, carbon storage, energy and water fluxes, N fixation and N cycling. Future climate feedbacks depend on how quickly vegetation patterns change in response to regional warming. Predicting such changes is difficult, however, because they are not simply a function of shifts in the climate envelope of suitable temperature and moisture; expansion is influenced by interacting factors, including dispersal, recruitment, soil temperature, hydrology, biogeochemical cycling, edaphic characteristics, disturbance, and herbivory. We are synthesizing literature on known controls and rates of change in shrub cover, including a comparison of how arctic dynamic vegetation models (DVMs) incorporate shrub dynamics and how their results for future scenarios differ. We present a summary of our synthesis to date and a table that compares and contrasts arctic DVMs and their treatment of shrub dynamics.

Poster #1-17

Non-Growing Season Plant and Soil Biogeochemistry in High-Latitude Tundra have Large Effects on Plant Nutritional Status and Carbon Budgets

William J. Riley[1*], Nicholas J. Bouskill[1], Robert F. Grant[2], Zelalem Mekonnen[1], Jinyun Tang[1], and Qing Zhu[1]

[1]Climate and Ecosystem Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Department of Renewable Resources, University of Alberta, Edmonton, Alberta, Canada

Contact: wjriley@lbl.gov

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

High-latitude permafrost ecosystems store large amounts of organic carbon, primarily because low temperatures hinder decomposition. For high-latitude systems, land models must represent the dominant nutrient (i.e., nitrogen (N) and phosphorus (P)) controls on the C cycle to predict C-climate interactions over the 21st century. Observations in high-latitude, including at the NGEE Arctic site near Barrow (recently renamed Utqiaġvik), AK and alpine systems indicate that plant activity belowground continues well past aboveground senescence. We analyzed non- growing season plant nutrient-uptake and plant-microbe competition at high latitudes, and estimate implications for decadal to centennial-scale Arctic C cycling. We apply two mechanistic ecosystem models (ELM, *ecosys*) that represent nutrient acquisition based on competitor traits (e.g., fine-root biomass, transporter density, V_{max}, affinities) to a high-resolution representation of BEO polygonal tundra and to a 25 km resolution representation of North American tundra. Our results indicate that plant nutrient uptake during the non-growing season have large effects on annual nitrogen losses and the long-term C balance of the Arctic.

Poster #18

Deep Look into Deep Permafrost: Impact of Warming on Microbial Functions

Neslihan Taş[1*], Yuxin Wu[1], Craig Ulrich[1], Baptiste Dafflon[1], Timothy Kneafsey[1], Susannah Tringe[2], Margaret Torn[1], Susan Hubbard[1], and Janet K. Jansson[3]

[1]Lawrence Berkeley National Laboratory
[2]DOE Joint Genome Institute
[3]Pacific Northwest National Laboratory

Contact: ntas@lbl.gov

BER Program: TES
Project: NGEE Arctic
Project Website: http://ngee-arctic.ornl.gov/

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. Especially the fate of carbon in deep permafrost, which is currently protected from the warming climate, is uncertain. In this project, we applied metagenomics and metatranscriptomics to determine the phylogenetic and functional changes in the deep permafrost microbiome from polygonal arctic tundra at the Barrow Environmental Observatory (BEO). We collected permafrost cores ranging from 0.5-3m in depth and analyzed over 200 samples along a transect containing high-, flat- and low-centered polygons in order to determine microbial responses to thaw. BEO permafrost layers were mainly populated with Actinobacteria. Besides depth, pH and changes in the material density were important drivers of microbial community structure. Metagenomes from different permafrost depths also showed elevated potential for CH_4 production in deeper layers while CH_4 production and oxidation potential was detected in near surface permafrost. Moreover deep permafrost layers were also populated by chemolithoautotrophic Alphaproteobacteria. We hypothesize that nutrients and available carbon in these layers are tightly regulated and recycled where permafrost increasingly becomes a CH_4 source with depth. 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 #19

Nitrate in a Changing Terrestrial Arctic

Jeffrey Heikoop[1*], Carli Arendt[2], Brent Newman[1], Rachael McCaully[2], Nathan Wales[1], Sanna Sevanto[1], David Graham[3], Cathy Wilson[1], and Stan Wullschleger[3]

[1]Earth and Environmental Sciences Division, Alamos National Laboratory, Los Alamos, NM
[2]Department of Marine, Earth and Atmospheric Science, North Carolina State University, Raleigh, NC
[3]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: jheikoop@lanl.gov

BER Program: TES
Project: NGEE Arctic
Project Website: http://ngee-arctic.ornl.gov/

In addressing questions of terrestrial Arctic wetting versus drying, the NGEE Arctic project has observed relationships between nitrate concentration and soil moisture. For example, in the drier centers and rims of high-, flat- and low-centered polygons in the Barrow Environmental Observatory (BEO) nitrate concentrations are significantly elevated (up to 34 mg/l). In surrounding saturated sediments nitrate concentrations are typically below detection. Nitrate concentrations were particularly high in high-centered polygons related to recent human disturbance outside the BEO (up to 88 mg/l), suggesting rapid increases in nitrate production associated with geomorphic change. Similar patterns were observed in microtopographic features at the NGEE Teller site in the Seward Peninsula. There, degraded peat plateaus represent microtopographic highs with lower soil moisture and detectable nitrate concentrations, whereas surrounding saturated soils have nitrate levels below detection. Nitrate concentrations and moisture content in peat plateau sediments were similar to those found in low- and flat-centered polygons in the BEO, despite being associated with very different vegetation communities. Moisture is clearly a first order control on soil nitrate concentrations at the BEO and Teller watershed. Drier, more oxic, environments are favorable for nitrate production from mineralization and accumulation of atmospheric nitrate inputs, with concentrations modified by demand from primary producers. Our studies at the Kougarok site, however, have shown no correlation between nitrate and soil moisture content in alder stands where nitrogen fixation introduces new nitrogen into soils. Moreover, initial results from this site suggest that interflow can transport nitrate downslope away from areas of production. Thus, alder encroachment can increase nitrate availability in downslope areas. Within the BEO, we also find that the relationship between nitrate and soil moisture is complex. The rims of drained thaw lake basins and drier drainage slopes, despite having lower moisture content, do not always have elevated nitrate concentrations, possibly due to vegetation differences. Moisture content, quantity and quality of organic matter, microbial community composition, vegetation, and hydrology are all potential controls on nitrate contents in Arctic soils, with different controls dominant in different environments. Each of these factors is expected to change as permafrost thaws, landscapes evolve, vegetation communities shift (e.g. shrubification), moisture is redistributed across the landscape. A fuller understanding of the factors that control nitrate (and other nutrients) in different permafrost environments will be essential in predicting future nitrate levels and attendant feedbacks on Arctic carbon cycling.

Poster #1-20

Stimulation of Anaerobic Organic Matter Degradation by Nitrogen Addition in Tundra Soils

Michael Philben[1*], Jianqiu Zheng[2], David Graham[2], Markus Bill[3], Jeffrey Heikoop[4], Stan Wullschleger[1], and Baohua Gu[1]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[3]Earth and Environmental Sciences, Lawrence Berkeley National Laboratory, Berkeley, CA
[4]Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM

Contact: philbenmj@ornl.gov

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

Nitrogen (N) availability in arctic soils is hypothesized to increase with warming due to accelerated mineralization of organic N from soil organic matter and the release of labile N from thawing permafrost. The potential for increased N availability to increase plant growth and associated C inputs to the soil is being incorporated into biogeochemical models. However, soil microorganisms will also compete for the additional N, which could stimulate their growth and increase CO_2 and CH_4 emissions via organic matter decomposition. We investigated the effects of N addition on anaerobic organic matter degradation through both field and lab-based experiments. In the field experiment, we injected a solution of ^{13}C- and ^{15}N-labeled glutamate 35 cm below the soil surface in a tundra soil near Nome, Alaska, and observed the resulting changes in porewater geochemistry and dissolved greenhouse gas concentrations. In the lab experiments, we added either a single pulse or a continuous injection of glutamate to an anoxic column filled with soil collected from the same field site. In the field experiment, free glutamate was detected one hour after the tracer injection but the concentration rapidly declined, and the ^{15}N label was recovered as total dissolved N in only small amounts until 62 hours after the injection. These results suggest that most of the added N was rapidly assimilated, consistent with microbial N limitation, which was followed by a later phase of mineralization or release as dissolved organic N. Both lab experiments also exhibited an initial phase of glutamate loss following the injection, consistent with microbial assimilation. We also observed increased concentrations of dissolved CH_4 during the field experiment, and Fe(II) during both the lab and field experiments, indicating stimulation of methanogenesis and Fe(III) reduction. Increasing concentrations of low molecular weight organic acids such as acetate and propionate suggests that N addition stimulated the decomposition and fermentation of more complex organic matter, likely as a result of relieved substrate limitation for anaerobic respiration. However, the resulting organic matter degradation appeared selective: while the total dissolved organic carbon (DOC) concentration declined by as much as 50% during the field experiment, there was no change in the aromatic DOC fraction as indicated by UV-Vis absorbance, resulting in an increase of specific UV absorbance ($SUVA_{254}$). Together, these results indicate that increasing N availability in tundra soils could accelerate warming-induced CO_2 and CH_4 production by relieving N limitation of fermenting microorganisms.

Poster #1-21

Modeling Anaerobic Soil Organic Carbon Decomposition in Arctic Polygon Tundra: Insights into Soil Geochemical Influences on Carbon Mineralization

Jianqiu Zheng[1], David E. Graham[1,3*], Scott L. Painter[2,3], Peter E. Thornton[2,3], Baohua Gu[2], and Stan D. Wullschleger[2,3]

[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[3]Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: grahamde@ornl.gov

BER Program: TES
Project: NGEE Arctic
Project Website: http://ngee.ornl.gov

Rapid warming of Arctic ecosystems exposes soil organic matter (SOM) to accelerated microbial decomposition, potentially leading to increased emissions of carbon dioxide (CO_2) and methane (CH_4) that have a positive feedback on global warming. The fate of permafrost carbon is determined in large part by soil moisture, and a significant portion of carbon may thaw in wet, anoxic conditions. Current estimates of the magnitude and form of carbon emissions from Earth system models include significant uncertainties, because the models do not explicitly represent anaerobic carbon decomposition. We coupled modeling principles developed in different disciplines, including a thermodynamically based microbial growth model for methanogenesis and iron reduction, a pool-based model to represent upstream carbon transformations, and a humic ion-binding model for dynamic pH simulation to build a more versatile carbon decomposition model framework that can be applied to soils under varying redox conditions. This new model framework was parameterized and validated using synthesized anaerobic incubation data from permafrost-affected soils along a gradient of fine-scale thermal and hydrological variabilities across Arctic polygonal tundra. The model accurately simulated anaerobic CO_2 production and its temperature sensitivity using data on labile carbon pools and fermentations rates as model constraints. Modeling and synthesis results demonstrate that CH_4 production is strongly influenced by water content, pH, methanogen biomass, and presence of competing electron acceptors, resulting in high variability in its temperature sensitivity. This work provides new insights into the interactions of SOM pools, temperature increase, soil geochemical feedbacks, and resulting CO_2 and CH_4 production. The proposed anaerobic carbon decomposition framework presented here builds a mechanistic link between soil geochemistry and carbon mineralization, making it applicable over a wide range of soils under different environmental settings. Data sets can be found at http://dx.doi.org/10.5440/1168992, http://dx.doi.org/10.5440/1393836, and http://dx.doi.org/10.5440/1288688

Poster #1-22

Simulating the Impact of Regional Subsidence and Polygonal Ground Degradation on Arctic Permafrost Hydrology

Ethan Coon[1*], Scott Painter[1], Ahmad Jan[1], David Moulton[2], Cathy Wilson[2], and Adam Atchley[2]

[1]Environmental Sciences Division, Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Los Alamos National Laboratory, Los Alamos, NM

Contact: coonet@ornl.gov

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

Many permafrost-affected regions in the Arctic manifest a polygonal-patterned ground, which is characterized by large carbon stores and vulnerability to climate change. In these areas, warming temperatures drive melting of ice wedges and distributed bulk ice, resulting in systematic polygon degradation and subsidence, and thawing of the underlying carbon-rich soils, resulting in increased decomposition rates. Predicting the fate of this carbon is difficult. The system is controlled by complex, nonlinear physics coupling biogeochemistry, thermal-hydrology, and geomorphology, and there is a strong spatial scale separation between microtopography (at the scale of an individual polygon) and the scale of landscape change (at the scale of thousands of polygons). The Next Generation Ecosystem Experiment – Arctic has developed a multi-scale, process-rich modeling strategy for understanding how geomorphology and thermal-hydrology combine to determine the hydrologic environment as these soils thaw. Over the life of the project, physics-based models were developed, and scaling strategies to move from fine-scale, mechanistic models of individual polygons to intermediate-scale models over many polygons have been developed. Here we demonstrate how the resulting multi-scale strategy can be used to study the interplay between thermal-hydrology and geomorphology. It has long been hypothesized that regional subsidence, caused by melting of distributed bulk ice, can decrease porosity, resulting in apparently wetter soil. Polygon degradation has been shown to increase the connectivity of flow pathways, resulting in better drainage and apparently drier soil. We demonstrate that our model can represent those effects individually, and begin to address how the competing effects collectively determine the evolution of polygonal tundra hydrology in a warming climate.

Poster #1-23

Flow and Transport Characteristics of Ice-wedge Polygons

Nathan Wales[1*], Brent Newman[1], Jesus Gomez-Valez[2], Cathy Wilson[1], Daniil Svyatsky[1], Julie Jastrow[3], and Stan Wullschleger[4]

[1]Los Alamos National Laboratory, Los Alamos, NM
[2]New Mexico Institute of Mining and Technology, Socorro, NM
[3]Argonne National Laboratory, Argonne, IL
[4]Enivironmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: bnewman@lanl.gov

Program: TES
Project: NGEE Arctic
Project Website: http://ngee-arctic.ornl.gov/

In an effort to better understand flow and transport processes in ice-wedge polygons and provide data to inform permafrost models, such as the Arctic Terrestrial Simulator (ATS), tracer studies were conducted on a low- and high-centered polygon in the Barrow Environmental Observatory (BEO). With this experiment we found that tracer breakthrough was highly heterogeneous in both polygons. Horizontal flux occurred in more locations and at higher rates in the low-centered polygon than in the high-centered polygon. Hydraulic connectivity was shown to exist between polygon centers and troughs. Results also suggest that most of the tracer mass still remains in polygon centers. In its current state, the ATS does not represent heterogeneous horizontal transport of tracer as observed in the field experiment. While time series sampling for the field experiment has concluded, results of the experiment have given rise to new questions. Moving into NGEE Arctic Phase 3, key factors have been identified for further investigation. We plan to investigate the influence of active layer heterogeneity on tracer transport. For example, we speculate that ice lenses play a role in heterogeneity of tracer transport and the higher occurrence of tracer breakthrough observed in the low-centered polygon. Soil properties also likely influence tracer distribution. Understanding soil structure, stratigraphy, and cryoturbation could potentially provide insight into the existence of preferential flow paths or systems of secondary porosity and their influence on tracer transport. Finally, an estimate of tracer mass remaining in polygon centers is needed to better understand the residence time of tracer in polygon systems. To answer these questions, we are considering a several paths forward including: 1) initializing ATS simulations with soil cross-section data derived from J. Jastrow's soil pits on the BEO, 2) end of winter coring of the tracer polygons and 3) trenching both tracer polygons. Simulations with better representation of cryoturbation features would help us diagnose the role of soil heterogeneity in our observations, and cores and trenches would provide site specific data to close our tracer mass balance for the experiments. Current tracer results are being used to make improvements to the ATS model and Phase 3 investigations will also serve to improve ATS representation of flow and transport in ice-wedge polygons.

Poster #1-24

Investigations of Topographic Control on Thermokarst Development and the Ground Thermal Regime in Ice Wedge Polygons using the Advanced Terrestrial Simulator

Charles Abolt[1*], Michael Young[1], Adam Atchley[2], Dylan Harp[2], and Ethan Coon[3]

[1]University of Texas at Austin, Austin, TX
[2]Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM
[3]Environmental Sciences Division, Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: chuck.abolt@beg.utexas.edu

BER Program: TES
Project: NGEE Arctic
Project Website: http://ngee-arctic.ornl.gov/

Permafrost degradation in ice wedge polygon terrain has accelerated in the last three decades, resulting in drastic changes to tundra hydrology which may impact rates of soil organic carbon mobilization. The goal of this research is to determine to what extent the near surface thermal regime, and hence the vulnerability of the upper permafrost, may be controlled by surface topography in ice wedge polygons. The central hypothesis is that energy is preferentially transferred into the polygon subsurface in summer at low, wet zones (such as low-centered polygon centers and troughs), then released to the atmosphere in winter through elevated zones (such as rims) that are less insulated by snowpack. Disturbance to the approximate balance between these seasonal energy fluxes may help explain the onset and development of thermokarst. In this work, we present a numerical model of thermal hydrology in a low-centered polygon near Prudhoe Bay, Alaska, constructed within the Advanced Terrestrial Simulator, a state of the art code that couples a meteorologically driven surface energy balance with equations for surface and subsurface conservation of mass and energy. The model is calibrated against a year of daily ground temperature observations throughout the polygon and used to quantify meter-scale zonation in the subsurface thermal budget. The amount of relief in the rims and the trough of the simulated polygon is then manipulated, and simulations are repeated including a pulse of one warm year, to explore the extent to which topography may influence the response of permafrost to increased air temperatures. Results suggest that nearly 80% of energy entering the ground at the trough during summer may be released back to the atmosphere through the rims in winter, substantially enhancing cooling in the ice wedge, and implying that cracking may be impeded as polygon rims erode. Active layer thickness is modestly impacted by rim size, because the subsurface in polygons with larger rims is colder at the start of the thaw season. As troughs deepen, ice wedge degradation may be accelerated by positive feedbacks, because inundated troughs sustain thicker active layers. The results expand upon current conceptual understanding thermokarst development in polygonal terrain and shed light on nonlinear changes to Arctic hydrology driven by a warming climate.

Poster #1-25

Modeling Drivers of Discontinuous Permafrost on a Hillslope Transect

Elchin Jafarov[1*], Ethan Coon[2], Dylan Harp[1], Cathy Wilson[1], Scott Painter[2], Adam Atchley[1], and Vladimir Romanovsky[3]

[1]Los Alamos National Laboratory, Los Alamos, NM
[2]Environmental Sciences Division, Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[3]University of Alaska Fairbanks, Fairbanks, AK

Contact: elchin@lanl.gov

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

Recent studies observed increase in the discharge of Arctic rivers; some hypothesize that this increase is due to thawing and discontinuous permafrost. Understanding conditions resulting in the loss of permafrost, along with the path from continuous permafrost to discontinuous permafrost to seasonally frozen ground, is important to test this hypothesis. In particular, how will changes in permafrost thermal conditions affect subsurface flow pathways? An open talik is a thawed zone extending through the entire permafrost layer. Open taliks play a critical thermal hydrologic role of water redistribution and heat conductance anomalies, which is likely amplified in sloping landscapes. Understanding how local environmental conditions, such as snow distribution, influences talik formation and the thermal hydrologic response of talik formation is necessary to predict complex thermal, hydrologic, and carbon cycle responses in Arctic systems. We used the coupled surface/subsurface permafrost hydrology model ATS (Advanced Terrestrial Simulator) version 0.86 to model an open talik formation by preferentially distributing snow depth along the surface of an inclined modeling domain, representative of a hillslope transect. We used de-trended meteorological data to test talik formation under preferentially distributed snow depth. To test how permafrost thickness affects talik formation we setup the model with five different permafrost thickness ranging from 18m to 45m. For three out of five cases the model developed an open talik allowing water from the seasonally thawed near-surface to be mixed with sub-permafrost waters. In all cases the total water storage in the modeling domain increased. This work indicates that variability in snow depth due to landscape properties can drive significant changes in permafrost hydrology.

Poster #1-26

Modeling the Impacts of Fire on Surface Energy and Land-Atmosphere Carbon Exchange Across Alaska

Zelalem Mekonnen[1*], William J. Riley[1], James T. Randerson[2], and Robert F. Grant[3]

[1]Climate and Ecosystem Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Department of Earth System Science, University of California, Irvine, CA
[3]Department of Renewable Resources, University of Alberta, Edmonton, Alberta, Canada

Contact: zmekonnen@lbl.gov

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

Fire is an important driver of the carbon cycle across northern ecosystems. The impact of recent and predicted changes in fire regimes on net carbon exchange is uncertain. Here we applied an ecosystem model, *ecosys*, to examine the effects of fire on surface energy and land-atmosphere carbon exchanges across selected sites in Alaska. The model was prescribed with known fire vs. non-fire (control) events across the selected sites. Changes in surface energy budget during fire chronosequence were modeled to drive differences in soil temperature across sites. Soil temperature was warmer in the post-fire vs. the control during summer and spring but colder during winter. An average of ~30 % reduction in ecosystem net radiation (*Rn*) was modeled in the postfire vs. the control sites. Greater differences in *Rn* and sensible heat during spring vs. fall were modeled from differences in surface albedo. Modeled heterotrophic respiration (*Rh*) was higher in the postfire sites in spring from earlier soil warming. However, lower *Rh* was modeled during fall and winter from soil cooling as a result of lesser insulation of the soil surface layer after fire. Emissions from fire was modeled to result in carbon losses that offset from 20 to >100% of the decadal carbon sinks across the selected sites.

Terrestrial Ecosystem Science

Next Generation Ecosystem Experiments (NGEE): Tropics

Poster #9-6

The Next Generation Ecosystem Experiments (NGEE)-Tropics Overview

Jeffrey Chambers[1*], Deb Agarwal[1], Stuart Davies[2], Rosie Fisher[3], Michael Keller[4], Charlie Koven[1], Lara Kueppers[1], Ruby Leung[5], Nate McDowell[5], Rich Norby[7], Alistair Rogers[8], and Chonggang Xu[6]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Smithsonian Tropical Research Institute, Washington, DC
[3]National Center for Atmospheric Research, Boulder, CO
[4]USDA Forest Service, International Institute of Tropical Forestry, San Juan, PR
[5]Pacific Northwest National Laboratory, Richland, WA
[6]Oak Ridge National Laboratory, Oak Ridge, TN
[7]Los Alamos National Laboratory, Los Alamos, NM
[8]Brookhaven National Laboratory, Upton, NY

Contact: jchambers@lbl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Tropical forests cycle more CO_2 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. The Next Generation Ecosystem Experiments (NGEE)-Tropics is a large multi-institutional research project funded by BER and aimed at improving ESM 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 is developing a transformational, process-rich model framework (the Functionally Assembled Terrestrial Ecosystem Simulator–FATES) where the responses and feedbacks of tropical forests to a changing climate are modeled at the scale of a next generation ESM grid cell.

Research thus far has focused on developing an improved understanding and model representation of key tropical forest processes including: responses to changing temperature, precipitation, and atmospheric CO_2; disturbance and land-use change; and heterogeneity in belowground processes. FATES has been successfully integrated into DOE's Energy Exascale Earth System Model (E3SM), and further model development and measurement activities are being integrated at pilot study field sites in Puerto Rico, Brazil, and Panama. A data synthesis and management framework has been developed to provide data products via a community portal.

Poster #9-7

Variation in the Representation of Photosynthesis in CMIP5 Terrestrial Biosphere Models

Alistair Rogers[1*], Shawn Serbin[1], and Anthony Walker[2]

[1]Brookhaven National Laboratory, Upton, NY
[2]Oak Ridge National Laboratory, Oak Ridge, TN

Contact: arogers@bnl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Estimates of gross primary productivity by terrestrial biosphere models (TBMs) rely on accurate model representation of leaf level photosynthesis. We have used a modular modelling code to enable a process-level systems analysis of the representation of leaf level photosynthesis for an evergreen broadleaved tropical plant functional type. At the heart of many TBMs is the Farquhar, von Caemmerer and Berry (FvCB) model of C3 photosynthesis. We coded the TBM specific structure and parameterization used to represent the different flavors of the FvCB formulation in eight of the TBMs that were included in the fifth coupled climate carbon cycle model intercomparison project (CMIP5). Using the multi-assumption architecture and testbed (MAAT) we simulated the response of CO_2 assimilation to irradiance, temperature, vapor pressure deficit and carbon dioxide concentration for the various stock TBM configurations. The resulting plots of these simulations revealed dramatic model divergence. We then conducted a stepwise unification of model structural and parametric assumptions which demonstrated the influence of key PFT specific parameters such as the maximum carboxylation rate, maximum electron transport rate and maximum triose phosphate utilization rate. Even with identical PFT specific parameterization there was still marked model divergence that was dominated by model assumptions associated with identification of the biochemical process limiting CO_2 assimilation, transport of CO_2 to the site of carboxylation, kinetic constants associated with CO_2 fixation and model representation of electron transport. These results highlight the importance of understanding the effect of model configuration on leaf level carbon assimilation and identify possible explanations for model diversity associated with highly integrative model outputs such as net ecosystem exchange and carbon storage.

Poster #9-8

A Convergent Spectroscopy-based Approach for Vcmax across Leaf Age and Growth Environments

Jin Wu[1*], Alistair Rogers[1], Loren Albert[2], Kim Ely[1], Neill Prohaska[3], Brett Wolfe[4], Raimundo Cosme Oliviera[5], Scott Saleska[3] and Shawn Serbin[1]

[1]Environmental & Climate Sciences Department, Brookhaven National Laboratory, Upton, NY
[2]Institute of Environment and Society, Brown University, Providence, RI
[3]Department of Ecology and Evolutionary Biology, University of Arizona, Tucson, AZ
[4]Smithsonian Tropical Research Institute, Gamboa, Panama
[5]Embrapa Amazonia Oriental, Santarem, Brazil

Contact: jinwu@bnl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Understanding the temporal patterns of leaf photosynthetic capacity (the maximum rate of RuBP carboxylation, Vcmax) is critical for determining photosynthetic seasonality and the controls over terrestrial carbon, water, and energy fluxes. However, an efficient method for predicting of Vcmax using the spectroscopy approach across space and time is still lacking. Here, we leverage previous studies which have successfully linked leaf spectroscopy to leaf Vcmax and leaf age respectively, with a specific goal to explore the potential use of leaf spectroscopy as a general means to rapidly estimate and monitor temporal changes in Vcmax. Here we address three questions: (1) whether there exists a convergent relationship between leaf Vcmax and spectroscopy across tropical forest sites, species, leaf age, and growth environments, (2) how well can the spectroscopy approach predict temporal variation in leaf Vcmax compared with the field observed Vcmax-age relationship, and (3) how do spectroscopy-derived Vcmax-age relationships vary across species and growth environments? To address these questions, we used field data collected in two tropical evergreen forests in Panama (n=15 species) and one in Brazil (n=5 species). These data include detailed field measurements of leaf age, full range reflectance spectroscopy (i.e. 350-2500 nm), Vcmax (derived from leaf gas exchange measurements), and growth environments (i.e. sun vs. shade). Our results suggest that leaf reflectance spectroscopy can accurately predict leaf Vcmax at the fully expanded age status across tropical forest sites ($R^2=0.7$, $p<0.001$). However, this single-age spectra-Vcmax relationship requires recalibration when it is applied to broader demographic classes (i.e. young, expanding leaf age class). Combining spectroscopy-based leaf Vcmax with spectroscopy-based leaf age, we further constructed the Vcmax-age relationship, which agreed well with field observations, suggesting that the spectroscopy technique is able to capture the temporal trajectories of Vcmax across the entire life cycle of leaves. This will aid development of remote sensing methods to characterize temporal variation of leaf photosynthetic metabolism across spatial and temporal scales, and enable remotely based parameterization and evaluation of Earth system models.

Poster #9-9

Drought Impacts on Non-structural Carbohydrate Dynamics in Tropical Forests

Turin Dickman[1*], Nate McDowell[2], Shawn Serbin[3], Kim Ely[3], Brett Wolfe[4], Matteo Detto[4], Jin Wu[3], Charlotte Grossiord[1], Adam Collins[1], Sean Michaletz[5], Joe Wright[4], Alistair Rogers[3], and Chonggang Xu[1]

[1]Earth & Environmental Science Division, Los Alamos National Laboratory, Los Alamos, NM
[2]Earth Systems Analysis & Modeling, Pacific Northwest National Laboratory, Richland, WA
[3]Environmental & Climate Sciences Department, Brookhaven National Laboratory, Upton, NY
[4]Smithsonian Tropical Research Institute, Balboa Ancon, Panama, Republic of Panama
[5]Department of Ecology and Evolutionary Biology, University of Arizona, Tucson, AZ

Contact: lee@lanl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov

Non-structural carbohydrates (NSC) provide a measure of the carbon supply available to support tree respiration, growth, and defense. Support for a role of carbon starvation -- or depletion of NSC stores -- in drought induced tree mortality is varied without consensus for the tropics. The 2016 ENSO drought provided a unique opportunity to capture drought impacts on tropical forest carbohydrate dynamics. To quantify these impacts, we collected monthly NSC samples, in conjunction with diurnal leaf water potential, gas exchange, and leaf spectral measurements, across a rainfall gradient in Panama for the duration of the ENSO.

Foliar NSC depletion did not progress with drought duration as predicted, but showed little variation over course of the ENSO and across sites. We observed high variability in foliar NSC among species, however, with structural traits accounting for some of this variation. Leaf mass per area correlated positively with foliar NSC, consistent with the increase in leaf dry mass as sugars accumulate. Degree of isohydry was also predictive of NSC, with lower branch soluble sugars in relatively isohydric species (those that maintain constant leaf water potential as soil water potential declines) and higher branch soluble sugars in relatively anisohydric species (those that allow leaf water potential to decline progressively as soil water potential declines), possibly due to the need for osmoregulation to maintain water potentials under dry conditions. These results emphasize the importance of trait-based modeling to capture species variation in NSC. Significant, but weaker, relationships were also found between foliar NSC and photosynthesis, leaf water potential, and leaf temperature. These findings will be used to evaluate whether the current implementation of carbohydrate dynamics and carbon starvation in FATES is capturing observed trends in tropical forest carbon allocation and mortality, and to tune model parameters for improved predictive capability.

Given the logistical difficulty of accurately sampling and measuring NSC, particularly in the tropics where rapidly freezing samples to halt enzymatic activity is particularly challenging, we took advantage of our coincident NSC and leaf spectra measurements to explore the potential for remotely sensing foliar NSC. Our Partial Least Squares Regression (PLSR) approach yielded promising models for predicting foliar soluble sugars and starch with broadband spectral data. This study demonstrates the potential for rapid and accurate estimation of these difficult to measure foliar traits that are key for understanding and accurately representing canopy carbon dynamics in earth systems models (ESMs).

Poster #9-10

The Pan-tropical Response of Soil Moisture to El Niño

Kurt Solander[1*], Brent Newman[1], Carter Berry[2], Damien Bonal[3], Rolando Célleri[4], Bradley Christoffersen[5], Wouter Dorrigo[6], Ruby Leung[7], Nate McDowell[7], Gretchen Miller[8], Georgianne Moore[8], Robinson Negron-Juarez[9], Christian Stiegler[10], Brett Wolfe[11], and Chonggang Xu[1]

[1]Earth and Environmental Sciences, Los Alamos National Laboratory, Los Alamos, NM
[2]University of New Hampshire, Durham, NH
[3]French National Institute for Agricultural Research, Paris, France
[4]University of Cuenca, Cuenca, Ecuador
[5]University of Arizona, Tucson, AZ
[6]Vienna University of Technology, Vienna, Austria
[7]Earth Systems Analysis & Modeling, Pacific Northwest National Laboratory, Richland, WA
[8]Texas A&M University, College Station, TX
[9]Lawrence Berkeley National Laboratory, Berkeley, CA
[10]Georg-August-Universität Göttingen, Göttingen, Germany
[11]Smithsonian Tropical Research Institute, Panama City, Panama

Contact: ksolander@lanl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov

The 2015-16 El Niño event ranks as one of the most severe on record in terms of the sea surface temperature (SST) anomalies generated in the tropical Pacific Ocean. Corresponding global impacts on terrestrial hydrology were thus expected to rival, or even surpass, those of the 1997-98 severe El Niño event, which had SST anomalies that were similar in magnitude and extent. However, the terrestrial hydrologic response to a strong El Niño, even in those areas that are expected to receive well above or below normal precipitation during such events, is not always consistent. We investigate where the soil moisture response to severe El Niño events is strongest by highlighting areas in the humid tropics (-25° to +25° latitude) according to the Koeppen climate classification system that experience consistent changes in soil moisture magnitude and direction during the three most recent major El Niño events of 1982-83, 1997-98, and 2015-16. We use gridded data from the Global Land Data Assimilation System (GLDAS) where the soil moisture response is measured according to October to December (OND) and January to March (JFM) changes in volumetric soil moisture relative to the previous OND and JFM seasons. The strongest declines were found in South America and Oceania with a mean change of -42% and -31%, respectively, over both seasons. The strongest increase of 24% was observed in East Africa during JFM. Confidence in these estimates was assessed by comparing the 2015-16 El Niño soil moisture response from in- situ observations to modeled estimates from the GLDAS grid cells that encompassed those measurements. Our work improves the understanding of El Niño impacts on soil moisture estimates in models and offers insight on the expected spatial differences of these impacts to improve water resource management efforts for regions where changes are expected to be most severe.

Poster #9-11

Understanding the Control of Hydraulic Traits in Tropical Forests Using a Hydrodynamic Model within a Demographic Vegetation Model

Chonggang Xu[1*], Bradley Christoffersen[2], Ryan Knox[3], Liang Wei[1], Rosie Fisher[4], Charlie Koven[3], and Nate McDowell[5]

[1]Los Alamos National Laboratory, Los Alamos, NM
[2]University of Texas Rio Grande Valley, Edinburg, TX
[3]Lawrence Berkeley National Laboratory, Berkeley, CA
[4]National Center for Atmospheric Research, Boulder, CO
[5]Pacific Northwest National Laboratory, Richland, WA

Contact: cxu@lanl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Vegetation plays a key role in global carbon cycles and thus is an important component within the Earth system models (ESMs) to project future climates. A recent trend for ESM vegetation modeling is to incorporate size- and succession-stage-structured demographic models. These models make it feasible for more realistic representation of key processes that control vegetation dynamics. In this study, we reported a new hydrodynamics (HYDRO) model within the DOE- sponsored the dynamic vegetation model, the functionally assembled terrestrial simulator (FATES-HYDRO). The HYDRO model is built on the size and canopy structure representation within FATES and is expected to better capture the control of hydraulic traits in both vegetation dynamics and carbon/water fluxes. As the first step, we conducted a parameter sensitivity analysis using the distribution of biologically-interpretable and measurable plant hydraulic traits. We focused on tropical forests, where co-existing species have been observed to possess large variability in their hydraulic traits. We first assembled 10 distinct datasets of plant hydraulic traits of stomata, leaves, stems, and roots, determined the best-fit theoretical distribution for each trait, and linked these based on taxonomically-standardized species names to generate a rank correlation matrix, which quantified the degree of interspecific (between-species) trait-trait coordination. Our analysis showed that hydraulic traits that determine the soil-root connection and the stomata control are more important for dry periods, while hydraulic traits that determine the whole tree conductance are more importance for wet periods. We also linked the loss of hydraulic conductivity to tree mortality related to hydraulic failure and then compared the sensitivity of mortality to three hypothesized mechanisms: carbon starvation, hydraulic failure, and a combination of carbon starvation and hydraulic failure based on a d13c isotopic approach. Our preliminary results show that there is a substantial difference in the simulated mortality depending on the mortality mechanisms selected. Our analysis suggests that hydraulic traits could play an important role in carbon and water fluxes and vegetation dynamics in tropical forests and further measurements to capture the hydraulic control on stomata, root-soil interface and whole tree resistance could improve our prediction of future tropical forests within ESMs.

Poster #9-12

Carbon, Water, and Energy Land-Atmosphere Exchanges in Wet and Seasonally Dry Forests in the Amazon

Alessandro Araujo[1*], Fiona Carswell[2], Yadvinder Malhi[3], Scott Saleska[4], Lucy Hutyra[5], Humberto Rocha[6], Celso von Randow[7], George Vourlitis[8], and Gilberto Pastorello[9]

[1]Brazilian Agricultural Research Corporation (EMBRAPA), Belem, Brazil
[2]Landcare Research, Lincoln, New Zealand
[3]Oxford University Centre for the Environment, Oxford, UK
[4]University of Arizona, Tucson, USA
[5]Boston University, Boston, USA
[6]University of São Paulo, São Paulo, Brazil
[7]Brazilian National Institute for Space Research (INPE), São Paulo, Brazil
[8]California State University, San Marcos, CA
[9]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: alessandro.araujo@embrapa.br

BER Program: TES
Project: NGEE-Tropics (LBA/EMBRAPA Collaborator)
Project Website: https://ngee-tropics.lbl.gov/; http://lba2.inpa.gov.br/

For over two decades, the Large-Scale Biosphere-Atmosphere Experiment in Amazonia (LBA) has been studying surface fluxes between the atmosphere and the biosphere in the Amazon biome. A network of towers is used for micrometeorological measurements across climatic and ecological gradients. Observational data show different behaviors between the equatorial part of the Amazon in the North (wet) and the Southern part (seasonally dry). Mechanisms such as deep root systems and hydraulic redistribution are evolutionary strategies allowing vegetation to take advantage of increases in surface radiation during periods with lower precipitation. However, there seems to be a physiological limiting factor, given that in these drier periods there are parts of the Amazon where carbon assimilation and evapotranspiration increase, while in other parts this is not the case. Comparing and integrating observational results into modeling work, including some of these mechanisms, has improved the predictive capacity of the models. This poster will show some of these results and discuss ongoing and future work in the Amazon within the context of the LBA Program.

Poster #9-13

Optimal Crown Temperature of Basal Stem CO_2 Efflux in Canopy Dominant Trees in the Central Amazon

Kolby Jardine, [1,2*], Leticia Oliveira Cobello[2], Bruno Gimenez[2], Niro Higuchi[2], and Jeffrey Chambers[1,2,3]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]National Institute for Amazon Research (INPA), Manaus, Brazil
[3]Department of Geography, University of California Berkeley, Berkeley, CA

Contact: Kjjardine@lbl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Stem respiration is estimated to represent 20-30% of autotrophic respiration, but its response to environmental drivers like temperature remains unclear. Although respiration sources and CO_2 transport in the transpiration stream are known to increase with temperature, their combined influence on diurnal stem CO_2 efflux (E_S) in the tropics remain poorly understood.

In this study, we show that basal E_S (1.3 m) from three canopy dominant trees in a mature tropical ecosystem in the central Amazon is tightly correlated with crown temperature (27-31 m) over fast (5 min), medium (hourly), and diurnal time scales. Transient variations in daytime crown temperatures caused by the passing of clouds overhead were accompanied by rapid variations in basal E_S.

Elevated crown temperatures during the daytime were accompanied by high sap velocities and reduced basal E_S. In contrast, during the night and rainy conditions, crown temperatures and sap velocities reached minimum values while basal E_S reached maximum values.

The results show that E_S was depressed when crown temperatures exceed 24-28.5°C, potentially reflecting an optimum crown temperature where stem CO_2 sources reach a maximum relative to stem CO_2 sinks (e.g. transport in the transpiration stream). We suggest this optimal temperature may be useful as a new benchmark for land models that mechanistically link autotrophic respiration and transpiration. In contrast to current global models, which predict higher E_S with temperature, our results imply that warmer conditions lead to reduced E_S and increased transport in the transpiration stream, potentially enhancing internal CO_2 re-assimilation and consequently carbon use efficiency and photo-protection during climate warming.

Poster #9-14

Advancements in the Functionally Assembled Terrestrial Ecosystem Simulator (FATES): Functional Hypotheses, Software and Testbeds

Ryan Knox[1*], Charles Koven[1], Rosie Fisher[2], Jennifer Holm[1], Jacquelyn Shuman[2], Yi Xu[3,4], Maoyi Huang[3], Boris Faybishenko[1], Chonggang Xu[5], William Riley[1], Erik Kluzek[2], Shawn Serbin[6], Gautam Bisht[1], Bradley Christoffersen[7], Ben Andre[2], Lara Kueppers[1] and Jeff Chambers[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]National Center For Atmospheric Research, Boulder, CO
[3]Pacific Northwest National Laboratory, Richland, WA
[4]School of Geography, Nanjing Normal University, Nanjing, China
[5]Los Alamos National Laboratory, Los Alamos, NM
[6]Brookhaven National Laboratory, Upton, NY
[7]University of Texas Rio Grande Valley, Edinburg, TX

Contact: rgknox@lbl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

The Functionally Assembled Terrestrial Ecosystem Simulator (FATES) is a dynamic, size and age structured, trait-filtering vegetation model. This model is an application of the Model- Experiment (MODEX) framework of the NGEE-Tropics project. It is developed with a mission to assess how forest dynamics interact with water, carbon and nutrient cycles and their subsequent impacts on global ecosystem health and energy interests. In the past year FATES has been coupled to ELM, the land model of E3SM (Energy Exascale Earth System Model). FATES allows the E3SM code to move beyond bioclimatic constraints to better represent the impact of dynamic plant competition, vertically structured canopies, and disturbances effects on vegetation.

Various improvements and advancements have been contributed to the FATES model over its development phase with the NGEE-Tropics project, which are grouped into three areas: 1) New and competing functional hypotheses have been introduced to represent various alternative processes, such as allometric relationships, and the ability to turn on/off modules like logging, fire, hydraulics, and leaf-biophysics; 2) Software codes were improved to obtain stability, extensibility, reproducibility, testing, introspectability, readability, etc.; and 3) Functional improvements to the model to accommodate science objectives, testbeds of tropical sites of interest to NGEE-Tropics, which can be used to enable parameterization and evaluation of the model.

Poster #9-15

Forest Dynamics and Severe Convection in Amazonia

Robinson Negron-Juarez[1*], Daniel Magnabosco-Marra[2], Jennifer Holm[1], Geraldine Derroire[3], Bruno Herault[3], Ervan Rutishauser[4], Benoit Burban[5], Damien Bonal[5], Helene Muller-Landau[4], Stuart Davies[4], Danielle Christianson[1], Matteo Detto[6], Sami Rifai[7], Alessandro Araujo[8], Chris Peterson[9], Adriano Lima[10], Niro Higuchi[10], William Riley[1], and Jeffrey Chambers[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Max Planck Institute for Biogeochemistry, Jena, Germany
[3]Agricultural Research for Development (CIRAD), French Guiana
[4]Smithsonian Tropical Research Institute, Panama City, Panama and Washington, DC
[5]French National Institute for Agricultural Research (INRA), Paris, France
[6]Princeton University, Princeton, NJ
[7]Oxford University, Oxford, UK
[8]Brazilian Agricultural Research Corporation (EMBRAPA), Para, Brazil
[9]University of Georgia, Athens, GA
[10]Brazilian National Institute for Amazonian Research (INPA), Manaus, Brazil

Contact: robinson.inj@lbl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Mesoscale Convective Systems (MCS) produce severe rainfall in the Amazon. MCSs such as squall lines can produce strong descending winds that can uprooting or break trees. Although the cause (severe rainfall) and effect (tree mortality) relationship is understood, how this relationship affects forest dynamics at the regional scale has not been examined. Here, we shed light on this issue.

Poster #9-16

Using a Process-Based Model to Disentangle Hydraulic Trait Relationships in Observations of Tropical Trees

Thomas Powell[1*], Brett Wolfe[2], Charles Koven[1], Boris Faybishenko[1], and Lara Kueppers[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Smithsonian Tropical Research Institute, Smithsonian Institution, Panama City, Panama

Contact: tlpowell@lbl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

In recent decades a considerable amount of data on the hydraulic traits of tropical forest tree species have been accumulated. These data are used to understand the physiology of water transport and its variation across species, ecosystems and precipitation gradients. It has been postulated that in areas with variable precipitation, fundamental trade-offs among hydraulic traits must exist in order for coexistence of a diversity of plant functional types (PFTs) to occur. However, strong evidence from direct observations for such a trade-offs has been elusive. Therefore, we use a process-based terrestrial ecosystem model with mechanistic representation of water transport, the Ecosystem Demography model (ED2-hydro), to perform a controlled set of simulations that explore how trade-offs emerge among xylem hydraulic conductivity (Kx), xylem vulnerability (xylem-P50), stem capacitance (Cs), stomatal control (stomatal-P50) and rooting depth, enabling coexistence of multiple PFTs. ED2-hydro was forced with local meteorological drivers and soil conditions from Barro Colorado Island, Panama. ED2-hydro was parameterized with various combinations of Kx, xylem-P50, Cs, and stomatal-P50 in a large ensemble of simulations to identify robust trade-off relationships.

When all trait combinations that resulted in coexistence across all simulated PFTs are considered, none of the ED2-hydro hydraulic traits appear to be strongly correlated, which is similar to observations of species-averaged traits compared within and across tropical ecosystems. However, ED2-hydro predicts that strong trade-offs between hydraulic traits do exist, but they only emerge when the traits of individuals that are in direct competition with each other are compared. For example, in ecosystems with seasonally and inter-annually variable precipitation, an axis of coexistence between hydraulically-safe and hydraulically-efficient PFTs occurs where the difference in xylem-P50 is inversely proportional the ratio of Kx for safe versus efficient PFTs. The model also predicts that coexistence occurs under variable precipitation when only the rooting depth differs, while holding the other hydraulic traits equivalent across PFTs. Based on our results from ED2-hydro, we hypothesize that hydraulic traits are strongly coordinated among individuals growing in direct competition at the forest-gap scale. We also recommend a series of field measurements to test if the relationships predicted by this modeling framework promote coexistence between PFTs with alternative hydraulic strategies.

Poster #9-17

NGEE-Tropics Data Management and Products

Charuleka Varadharajan[1*], Gilberto Pasterello[1], Boris Faybishenko[1], Danielle Christianson[1], Val Hendrix[1], Bradley Christoffersen[2], Matteo Detto[3,4], Kolby Jardine[1], Robinson Negron-Juarez[1], Bruno Gimenez[5], Charlotte Grossiord[2], Thomas Powell[1], Luiza Maria Aparecido[7], Gretchen Miller[7], Georgianne Moore[7], Heidi Asbjornsen[8], Carter Berry[8], Damien Bonal[9], Jeffrey Warren[6], Brett Wolfe[3], Jeffrey Chambers[1,10], Lara Kueppers[1,10], Nathan McDowell[11], and Deb Agarwal[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Los Alamos National Laboratory, Los Alamos, NM
[3]Smithsonian Tropical Research Institute, Washington, DC, and Panama
[4]Princeton University, Princeton, NJ
[5]National Institute of Amazonian Research (INPA), Manaus, Brazil
[6]Oak Ridge National Laboratory, Oak Ridge, TN
[7]Texas A&M University, College Station, TX
[8]University of New Hampshire, Durham, NH
[9]INRA-UMR, French Guiana
[10]University of California, Berkeley, CA
[11]Pacific Northwest National Laboratory, Richland, WA

Contact: cvaradharajan@lbl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: http://ngee-tropics.lbl.gov

NGEE-Tropics generates and utilizes ecological, hydrological, and meteorological datasets from tropical forests in Central and South America for scientific analysis and model parameterization and benchmarking. The overall goals of the Data Management and Synthesis objective is to work with the project team to: 1) host all project data in a community accessible archive and publicly release those data with appropriate citation and usage information, 2) standardize data and metadata collection for cross-site comparison, 3) curate data collected by the project and help acquire external data to create modeling testbeds, and 4) create priority data products such as meteorological model drivers, processed data with Quality Assurance/Quality Control (QA/QC), and cross-cutting synthesized datasets. Project data are archived for internal use in the NGEE- Tropics Archive, which has a portal to upload and search for data packages. A public listing of all data shared publicly and with the team are available at http://ngt-data.lbl.gov/dois, where authorized users can download data. All NGEE-Tropics data will migrate to the ESS-DIVE archive in March 2019. A metadata reporting framework FRAMES was developed for reporting sensor-based observations, and enabling cross-site and cross-method comparison, data interpretability, and QA/QC. Six core NGEE-Tropics field sites in Brazil, Panama, and Puerto Rico, as well as collaborators, have used the metadata templates to submit data packages to the NGEE-Tropics Archive. The standardized FRAMES templates have been used to synthesize the sapflux measurements collected across 9 field sites during the 2015-2016 El Niño. The synthesized dataset includes data collected from independent field efforts and incorporated community input from over 20 researchers. There were several challenges involved in synthesizing and comparing the data, including the variety of sensors used, data formats, units, and processing methods. Other key data products include several rounds of QA/QC of meteorological model drivers for three sites in Panama (BCI, San Lorenzo, and Parque Metropolitano), including air temperature, relative humidity, solar radiation, barometric pressure, wind speed and wind direction. The QA/QC-ed datasets have already been used as input data for the Ecosystem Demography model (ED2-hydro) and FATES simulations. The meteorological drivers along with other project data and relevant external datasets are being assembled into testbeds to spin-up and validate model simulations.

Together, the NGEE-Tropics Data Management and Synthesis objecting is focused on the long- term preservation of project data, and also create data products required to transform diverse and complex ecohydrological data into scientific understanding.

Poster #9-18

Predictability of Tropical Vegetation Growth

Jiafu Mao[1*], Binyan Yan[2], Forrest M. Hoffman[3], Daniel M. Ricciuto[1], Xiaoying Shi[1], and Min Xu[3]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Jackson School of Geosciences, University of Texas, Austin, TX;
[3]Computer Science and Mathematics Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: maoj@ornl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Though many researches have examined the sensitivity of tropical terrestrial ecosystems to various environmental factors, the predictability of tropical vegetation growth has remained to be explored. Using latest fine spatial resolution remote-sensing Enhanced Vegetation Index (EVI) and sea surface temperature (SST) indexes from different ocean basins, we examined the predictability of tropical plant dynamics in response to SST and established empirical models with optimal parameters for the hindcast prediction. Three evaluation metrics were employed to assess model performance, including correlations between historical and predicted values, percentage of correctly predicted signs in EVI anomalies, and percentage of correct signs for extreme EVI prediction. Our findings reveal that three regions, mainly over arid or semi-arid areas, were associated with strong influences of SST on EVI. For example, the eastern South America was primarily controlled by the Atlantic Ocean SST index, with a leading time of 2-4 months. In terms of the correlations between predicted and observed EVI anomalies, 70.26% (South America), 80.48% (Africa), and 76.27% (SE Asia) vegetated areas were diagnosed to be significant ($p<0.05$). At about 60% chances, the statistical models could correctly predict the sign of EVI anomalies, and the predictability increased to nearly 100% when EVI was extremely abnormal. These results enhanced the prediction of tropical terrestrial ecosystem, especially at seasonal to annual scales. Moreover, the statistics-based metrics will facilitate the benchmarking of Earth system models regarding the response of tropical vegetation growth to key oceanic drivers.

Poster #9-19

Phosphorus Sorption to Tropical Soils with Relevance to Earth System Model Needs

Melanie Mayes[1*], Wesley Porter[1,2], Julia Brenner[1], Jana Phillips[1], Joanne Childs[1], Xiaojuan Yang[1], Rich Norby[1], and Erika Marín-Spiotta[3]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Department of Geosciences, Middle Tennessee State University, Murfreesboro, TN
[3]Department of Geography, University of Madison-Wisconsin, Madison, WI

Contact: mayesma@ornl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Many tropical soils are considered phosphorus (P) limited, so the extent to which tropical forests can meet future carbon sink demands is critically influenced by P availability. Mineral soils exert a key control over P availability by forming strong chemical bonds with the orthophosphate (PO_4^{3-}) molecule. Here, we used an existing archive of 24 tropical soils and performed equilibrium batch isotherm experiments involving 0.3 g of soil and 0.03 L of solution in concentrations ranging from 0 to 500 mg PO4-P per L. The prioritization of sorption to higher energy sites before lower energy sites resulted in a nonlinear isotherm that was represented by fitting the data to the Langmuir isotherm. Langmuir parameters consist of Q_{max} which represents the maximum sorption capacity of the soil, and K which represents a binding coefficient. Our Q_{max} values ranged from 734 to 3775 mg PO_4^-P per kg of soil (mg/kg) with a median of 2060 mg/kg. We found significant correlations between Q_{max} values and clay content, total P, and iron and aluminum oxide content. The Langmuir K parameter ranged from 0.015 to 0.285 L/mg with a median of 0.081 L/mg. We did not find correlations between Q_{max} or K with soil order, which likely reflects the small size of our database. In comparing our data with the 12 available literature values for Langmuir parameters, we found that Q_{max} values seemed highly influenced by the initial P concentrations, suggesting that some authors did not add sufficient P to reach the plateau sorption values represented by the Q_{max} parameter. We also identified fitting of the nonlinear equation using linearized equations, which is known to impart significant errors. Thus, we have significant concern about the available sorption data to parameterize Earth system models. Further experiments with soils from Puerto Rico are expanding our database of knowledge to enable more thoroughly-vetted parameters for use in Earth system models.

Poster #9-20

A Multi-Hypothesis Modeling Approach to Study Sub-Canopy Carbon Balance

Anthony Walker[1*], Rosie Fisher[2], Ryan Knox[3], Charlie Koven[3], Alistair Rogers[4], and Shawn Serbin[4]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]National Center for Atmospheric Research, Boulder, CO
[3]Environmental Sciences Division, Lawrence Berkley National Laboratory, Berkley, CA
[4]Environmental & Climate Sciences Department, Brookhaven National Laboratory, Upton, NY

Contact: walkerap@ornl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

The Functionally Assembled Terrestrial Ecosystem Simulator (FATES) simulates competition among age and size structured populations of multiple plant functional types. Competition is currently based on access to and use of light and water. Light competition occurs via a vertically structured canopy with an over-canopy that receives full sun at its top and a sub-canopy that, at its top, receives the light that penetrates the over-canopy. With the current set of assumptions within FATES, mortality rates appear to be high in the sub-canopy which affects FATES' ability to reproduce observed forest age and size structures. We assume that a proportion of these high mortality rates is caused by assumptions in how leaf scale photosynthesis and respiration are represented and parameterized within FATES and how those assumptions affect the carbon balance of leaves in the sub-canopy. To investigate the variability in leaf carbon balance at low light levels caused by process representation and parameterization we used the multi-assumption architecture and testbed (MAAT). MAAT automates the combination, generation, and execution of a model ensemble built with different representations of process. MAAT also incorporates a novel method to calculate a process representation sensitivity index. The process representation sensitivity index quantifies the variability in a model outcome caused by variability in process representation (including parameterization). MAAT and the process representation sensitivity index provides a flexible and rigorous framework for analyzing model sensitivity to process representation, parametric variability, and environmental variability. An initial assessment of the sensitivity of the modeled leaf carbon balance under low light and typical tropical forest environmental conditions will be presented. Processes investigated will include photosynthesis, respiration base rates, stomatal conductance, and the temperature response of biochemical rates.

Poster #9-21

Improving Modeling of Water Table Dynamics by Incorporating Plant Hydraulics and Hillslope Based Drainage Function

Yilin Fang[1*], Chang Liao[1], Ruby Leung[1], Nate Mcdowell[1], and Teklu Tesfa[1]

[1]Pacific Northwest National Laboratory, Richland, WA

Contact: ruby.leung@pnnl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Spatial variability in water available for plant water use has an important control on how tropical forests respond to drought. Previous simulations performed over the Asu catchment, 80 km northwest of Manaus in the Amazon using ELM and CLM-Parflow identified development needs for modeling surface and subsurface hydrology in Earth system models. First, the drought index formulation and the simplicity of treating root water uptake as a sink term in soil hydrology in ELM lack mechanistic representation of the interaction of soil-plant system. Second, comparison between the one-dimensional ELM and three-dimensional Parflow model simulations indicated the importance of lateral flow in controlling groundwater table dynamics. To address the limitation in representing hydrodynamics of the soil-plant system, two simulations were performed at Manaus using plant hydraulics model within ELM. The model captured the hydraulic lift in the dry season, which is an important mechanism to prevent top soil moisture from depletion. The simulations showed that plants experience some water stress in the dry season, but the reduction in water availability is small even in simulations with water table depths differing by 6 meters. To model lateral flow, we introduced a representation of lateral fluxes as a drainage function using hillslopes to represent subgrid variability. This approach enables a realistic representation of lateral flow processes and their impact on hydrological and surface energy fluxes, while keeping additional computational cost minimal for Earth system modeling.

Poster #9-22

Assessing Impacts of Selective Logging on Water, Energy, and Carbon Budgets and Ecosystem Dynamics in Amazon Forests Using the Functionally Assembled Terrestrial Ecosystem Simulator

Maoyi Huang[1*], Yi Xu[1,2], Marcos Longo[2,3], Michael Keller[3,4,5], Ryan Knox[6], Charles Koven[6], and Rosie Fisher[7]

[1]Atmospheric Sciences and Global Change Division, Pacific Northwest National Laboratory, Richland, WA
[2]School of Geography, Nanjing Normal University, Nanjing, China
[3]Embrapa Agricultural Informatics, Campinas, Sao Paulo, Brazil
[4]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA
[5]International Institute of Tropical Forestry, USDA Forest Service, Rio Piedras, Puerto Rico
[6]Earth & Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, CA
[7]Climate and Global Dynamics Laboratory, National Center for Atmospheric Research, Boulder, CO

Contact: maoyi.huang@pnnl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov

Tropical forest degradation from logging, fire, and fragmentation not only alters carbon stocks and carbon fluxes, but also impacts physical land-surface properties such as albedo and roughness length. 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. As a first step to address these limitations, we implemented a selective logging module into the Functional Assembled Terrestrial Ecosystem Simulator (FATES) and parameterized the model to reproduce the selective logging experiment at the Tapajos National Forest in Brazil. The model was spun up until it reached the steady state, and simulations representative of intact forest and various logging practices and intensity were benchmarked against available eddy covariance and field ecological measurements. Our results suggest that the model realistically characterizes most water and carbon fluxes and stocks, the forest structure and composition, and the ecosystem succession following disturbance. However, the current version of FATES overestimates water stress in the dry season therefore fails to capture seasonal variation in latent and sensible heat fluxes. We also observed a bias towards low stem density and leaf area when compared to observations, suggesting that improvements are needed to allow establishment of additional trees. The effects of logging were assessed by different logging scenarios to represent reduced impact and conventional logging practices, both with high and low logging intensities. The model simulations suggest that even though the degraded forests rapidly recover water and energy fluxes in one to three years compared with old-growth forests, the recovery times for carbon stocks, forest structure and composition are much longer (i.e., more than 30 years depending on logging practices and intensity) . 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 study lays the foundation to simulate land use change and forest degradation in FATES, leading the way to direct representation of forest management practices and regeneration in Earth System Models.

Poster #9-23

Drivers and Mechanisms of Tree Mortality in Moist Tropical Forests

Nate McDowell[1*], Craig Allen[2], Kristina Anderson-Teixera[3,4], Paulo Brando[5,6], Roel Brienen[7], Jeff Chambers[8], Brad Christoffersen[9], Stuart Davies[3], Chris Doughty[10], Alvaro Duque[11], Fernando Espirito-Santo[12], Rosie Fisher[13], Clarissa Fontes[14], David Galbraith[7], Devin Goodsman[15], Charlotte Grossiord[15], Henrik Hartmann[16], Jennifer Holm[8], Daniel Johnson[15], Abd. Rahman Kassim[17], Michael Keller[18,19,20], Charlie Koven[8], Lara Kueppers[8,21], Tomo'omi Kumagai[22], Yadvinder Malhi[23], Sean McMahon[3], Maurizio Mencuccini[24], Patrick Meir[25,26], Paul Moorcroft[27], Helene Muller-Landau[28], Oliver L. Phillips[7], Thomas Powell[8], Carlos Sierra[16], John Sperry[29], Jeff Warren[30], Chonggang Xu[15], and Xiangtao Xu[31]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]U.S. Geological Survey, Fort Collins Science Center, Los Alamos, NM
[3]Smithsonian Tropical Research Institute, Washington, DC
[4]Smithsonian Conservation Biology Institute, Front Royal, VA
[5]Woods Hole Research Center, Falmouth MA
[6]Instituto de Pesquisa Ambiental de Amazonia, Brasilia, Brazil
[7]University of Leeds, Leeds, UK
[8]Lawrence Berkeley National Laboratory, Berkeley, CA
[9]University of Texas Rio Grande Valley, Edinburg, TX
[10]Northern Arizona University, Flagstaff AZ
[11]Universidad Nacional de Columbia, Medellín, CO
[12]University of Lancaster, Lancaster, UK
[13]National Center for Atmospheric Research, Boulder, CO
[14]University of California, Berkeley, CA
[15]Los Alamos National Laboratory, Los Alamos, NM
[16]Max Plank Institute for Biogeochemistry, Jena, Germany
[17]Forest Research Institute Malaysia, Selangor, Malaysia
[18]International Institute of Tropical Forestry, USD, San Juan, PR
[19]Embrapa Agricultural Informatics, Brasilia, Brazil
[20]Jet Propulsion Laboratory, Pasadena, CA
[21]Energy and Resources Group, University of California, Berkeley, CA
[22]The University of Tokyo, Japan
[23]University of Oxford, UK
[24]University of Barcelona, Spain
[25]Australian National University, Canberra Australia
[26]University of Edinburgh, UK
[27]Harvard University, Cambridge
[28]Smithsonian Tropical Research Institute, Panamá City, Panamá
[29]University of Utah, Salt Lake City, UT
[30]Oak Ridge National Laboratory, Oak Ridge, TN
[31]Princeton University, Princeton, NJ

Contact: nate.mcdowell@pnnl.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Tree mortality rates appear to be increasing in moist tropical forests (MTFs) with significant carbon cycle consequences. We review the state of knowledge regarding MTF tree mortality, create a conceptual framework with testable hypotheses regarding the drivers, mechanisms, and interactions that may underlie increasing MTF mortality rates, and identify next steps for improved understanding and reduced prediction. Increasing mortality rates are associated with rising temperature and vapor pressure deficit, liana abundance, drought, wind events, fire, and possibly CO_2 fertilization-induced increases in stand thinning or acceleration of trees reaching larger, more vulnerable heights. The majority of these mortality drivers may kill trees in part through carbon starvation and hydraulic failure. The relative importance of each driver is unknown. High species diversity may buffer MTFs against large-scale mortality events, but recent and expected trends in mortality drivers give reason for concern regarding increasing mortality within MTFs. Models of tropical tree mortality are advancing representation of hydraulics, carbon, and demography, but require more empirical knowledge regarding the most common drivers and their subsequent mechanisms. We outline critical datasets and model developments required to test hypotheses regarding the underlying causes of increasing MTF mortality rates, and improve prediction of future mortality under climate change.

Poster #9-24

Preliminary Results from Intensive Annual Surveys of Tree Mortality and Damage in Tropical Forests

Gabriel Arellano[1*], Sarayudh Bunyavejchewin[2], Álvaro Duque[3], S. Christine Fletcher[4], I-Fang Sun[5], María Uriarte[6], Jess Zimmerman[7], and Stuart Davies[1]

[1]Center for Tropical Forest Science, Smithsonian Tropical Research Institute, Washington, D
[2]Forest Research Office, Dept. of National Parks, Wildlife and Plant Conservation, Bangkok, Thailand
[3]Universidad Nacional de Colombia, Medellín, Colombia
[4]Forestry and Environment Division, Forest Research Institute, Kuala Lumpur, Malaysia
[5]Dept. of Natural Resources and Environmental Studies, National Dong Hwa University, Hualian, Taiwan
[6]Dept. of Ecology, Evolution & Environmental Biology, Columbia University, New York NY
[7]Dept. of Environmental Sciences, University of Puerto Rico, Rio Piedras, Puerto Rico

Contact: gabriel.arellano.torres@gmail.com

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Individual tree mortality is a fundamental component of the history and fate of forests. It drives forest structure and dynamics, floristic composition, and carbon and nutrient cycles. However, there is a gap in our understanding of the causes underlying individual tree mortality, particularly in tropical forests. Tree damage often precedes individual mortality, but the amount and type of this has been poorly documented or it is difficult to detect/estimate during fieldwork done at several years intervals. As part of the NGEE-Tropics project the ForestGEO designed and implemented a series of annual surveys of tree mortality/damage on a subset of trees on some of the big permanent plots in the tropics. The plots that have started with these surveys include Barro Colorado Island (Panama, 8500 stems), Amacayacu (Colombia, 5400 stems), Khao Chong (Thailand, 5000 stems), Huai Kha Khaeng (Thailand, 5000 stems), Pasoh (Malaysia, 6000 stems) and Fushan (Taiwan, 5500 stems). The protocol includes stems of different sizes and covers a representative area of individual 25-52-ha plots. The variables assessed in each intensive survey were: alive/dead, standing/broken/uprooted, living length, remaining percentage of crown, crown illumination index, leaning degree, presence of heavy liana infestation, fungal presence, wound level (1 to 3), presence of canker or deformities (1 to 3 in size), presence of rotten trunk (1 to 3 in area), percentage of defoliation, and presence of leaf damage. Other data, like lightning damage, landslides and fire damage, were also recorded when possible. A reduced version of this protocol was used to evaluate all trees ≥10 cm dbh at Luquillo (Puerto Rico, 18000 stems), to assess the damage caused by Maria hurricane in September 2017. Using these standardized data, we present preliminary results and inter-site comparisons on tree mortality and damage.

Poster #9-25

The Panama Tropical Forest Model Testbed: Comprehensive, Integrated Datasets on Abiotic Drivers, Plant Functional Traits, Tree Demography, and Stand-Level Carbon and Water Pools and Fluxes

Helene Muller-Landau[1*], Liza Comita[1,2], Richard Condit[1,3], James Dalling[1,4], Stuart Davies[1,5], Daisy Dent[1,6], Matteo Detto[1,7], Jefferson Hall[1], Stephen Hubbell[1,8], Ryan Knox[9], Isabel Martinez[7], Ervan Rutishauser[1], Stefan Schnitzer[1,10], Ben Turner[1], Maria Natalia Umaña[2], Michiel van Breugel[1,11], Brett Wolfe[1], and S. Joseph Wright[1]

[1]Smithsonian Tropical Research Institute, Balboa, Ancon, Panama
[2]Yale University, New Haven CT
[3]Field Museum of Natural History, Chicago, IL
[4]University of Illinois, Urbana, IL
[5]Smithsonian National Museum of Natural History, Washington, DC
[6]University of Stirling, Stirling, Stirlingshire, UK
[7]Princeton University, Princeton, NJ
[8]University of California, Los Angeles, CA
[9]Lawrence Berkeley National Laboratory, Berkeley, CA
[10]Marquette University, Milwaukee, WI
[11]National University of Singapore, Singapore

Contact: mullerh@si.edu

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

The improvement of the representation of tropical forests in global vegetation models – a task widely recognized as critical to by DOE and the modelling community – depends crucially on the availability of appropriate datasets for parameterization and evaluation. Panama offers a comprehensive and integrated set of datasets that provide an unmatched model testbed for tropical forests, a testbed that has been further developed in recent years by NGEE-Tropics. Here, we present an overview of these datasets, and key results for relationships of interest for evaluating models at a variety of spatial and temporal scales and levels of organization. The study area spans natural rainfall gradients from <1500 mm to >6000 mm of rainfall per year, as well as extensive variation in soils, elevation, and land use history. High-quality, detailed microclimate data subject have been collected for decades at multiple locations. Local geology and soils are well-characterized. Leaf functional traits, wood density, seed mass, and height and crown allometries have been measured on hundreds of woody plant species. Over 150 long-term forest monitoring plots encompassing > 150 ha provide data on aboveground biomass, woody productivity, tree mortality, functional composition, and tree size distributions, and their relationship with climate, soils, and forest age. Seed traps and seedling censuses within these plots provide additional species-specific data on tree reproduction and recruitment and its interannual variation with climate. Eddy covariance quantifies high-resolution stand-level carbon and water fluxes to the atmosphere for > 5 years at 2 sites, and complementary measurements quantify soil CO_2 efflux, stem CO_2 flux, sap flux, runoff, and leaf phenology. Additional datasets quantify carbon fluxes in litterfall at weekly resolution for >30 years and annual tree growth from dendrometers for the last decade. Large-scale, long-term soil fertilization experiments and detailed measurements within them in old-growth and secondary forests provide an excellent platform for evaluating the ability of models to capture effects of soil nutrients. Additional large-scale, long-term experiments involve litter manipulation, soil warming, and the removal of lianas (woody vines). Censuses of liana stems and liana infestation status of trees, as well as liana removal experiments, enable analyses of how forest carbon budgets are affected by lianas – and demonstrates

that these effects are substantial, even though they are not yet captured in vegetation models. Altogether, central Panama offers a powerful model testbed to evaluate and improve model representation of tropical forests.

Poster #9-26

Distribution and Dynamics of Aboveground Biomass in Second Growth Tropical Forests of Puerto Rico

Douglas Morton[1*], Sebastian Martinuzzi[1,2], Michael Keller[3,4], Bruce Cook[1], and Eileen Helmer[5]

[1]NASA Goddard Space Flight Center, Greenbelt, MD
[2]University of Wisconsin, Madison, WI
[3]USDA Forest Service, International Institute of Tropical Forestry, San Juan, PR
[4]NASA Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA
[5]USDA Forest Service, Rocky Mountain Research Station, Fort Collins, CO

Contact: douglas.morton@nasa.gov

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/, https://glihtdata.gsfc.nasa.gov/puertorico/index.html

Large-scale agricultural abandonment in the 20th century created a mosaic of second growth forests across the island of Puerto Rico, distributed across a range of topographic, edaphic, and climatic conditions. Here, we combined forest inventory data and remote sensing products from the NASA Goddard Lidar, Hyperspectral, and Thermal (G-LiHT) Airborne Imager (www.gliht.gsfc.nasa.gov) to evaluate biomass accumulation in second growth forests across gradients of forest age, soils, and climate. A total of 78 Forest Inventory and Analysis (FIA) plots from the USDA Forest Service across the island, measured in 2016 and 2017, were combined with G-LiHT lidar data from 2017 to model biomass as a function of lidar-derived forest structure. Research plots from state and national forest lands were used to evaluate the lidar-biomass model for older second growth and mature forest types. In addition, 2017 G-LiHT data were compared with existing lidar coverage from 2011 and 2013 to estimate changes in canopy structure from branch and tree fall events over four to seven-year intervals. Lidar data offer a novel constraint on the size and frequency distributions of canopy change, in combination with estimated forest mortality from inventory plots. The information presented here is a key step towards improving the representation of tropical forest dynamics in ecosystem models, including the mechanics of forest succession that determine biomass accumulation in second- growth forests.

Poster #9-27

Quantifying Forest Degradation Using GLAS Lidar

Maria Hunter[1,2*], Michael Keller[2,3], Laerte Ferreira[4], and Leandro Leal Parente[4]

[1]Universidade Federal de Mato Grosso, Cuiabá, MT, Brazil
[2]United States Forest Service, International Institute of Tropical Forestry, Rio Piedras, PR
[3]NASA Jet Propulsion Laboratory, Pasadena, CA
[4]Universidade Federal de Goiás, Goiania, GO, Brazil

Contact: hunter.maria@gmail.com

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

In order to provide useful analysis and predictions of the global carbon cycle, Earth System models require information on forest structure. For demographic models, this requires tree number density according to size class. For regions of the Earth with detailed forest inventories, it is possible to initialize and test models based on inventory data. Unfortunately, large-scale, accurate, and current forests inventories are not available for vast regions of tropical forest. One potential source for future forest structure information is the GEDI Lidar that is expected to be deployed to the International Space Station in May 2019 and subsequent forest structure data as called for by the recent NASA Earth Science Decadal Survey. We explore lidar data from the GLAS Sensor onboard the ICESat satellite that operated from from 2003 to 2009. These distributions of power density in the retrieved lidar waveforms represent forest structure integrated over the lidar footprints (60 - 80 m diameter). These distributions (or metrics of the distributions) are compared for areas of intact forest in demarcated reserves with areas that have been identified as deforested or degraded by forest fire within Brazil. Active fire locations are from NASA's Fire Information for Resource Management Systems (FIRMS) for the period of 2003-2009 and are based on MODIS active fire signals. Higher resolution burn patterns that combine Landsat and MODIS data (such as the BDR algorithm or Imazon's burned area product) are also compared for limited time periods or areas as available.

Poster #9-28

Representing the Long-term Impacts of Forest Degradation in Amazon Forests in Dynamic Ecosystem Models

Marcos Longo[1,2*], Michael Keller[1,2,3], Maoyi Huang[4], and Douglas Morton[5]

[1]Embrapa Agricultural Informatics, Campinas, Sao Paulo, Brazil
[2]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA
[3]USDA Forest Service, International Institute of Tropical Forestry, Rio Piedras, Puerto Rico
[4]Atmospheric Sciences and Global Change Division, Pacific Northwest National Laboratory, Richland, WA
[5]NASA Goddard Space Flight Center, Greenbelt, MD

Contact: mdplongo@gmail.com

BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Deforestation and forest degradation are major drivers of changes in tropical forests and both contribute roughly equally to carbon stock depletion of tropical forest ecosystems worldwide. In the Amazon rainforest, the largest tropical forest in the world, deforestation rates have significantly decreased since 2005, but there is increasing evidence that forest degradation rates have not followed the downward trend. In contrast to deforested areas, sites that are disturbed by selective logging and understory fires — the main drivers of tropical forest degradation — retain some, albeit severely altered, forest structure and function. Most dynamic global vegetation models still have overly aggregated representation of the ecosystems, limiting their ability to properly represent the dynamics of tropical forest degradation. In this study we implemented a new selective logging module in the Ecosystem Demography Model (ED-2) to investigate the impact of a broad range of logging techniques, harvest intensities, and recurrence cycles on the long-term dynamics of Amazon forests. Model results were evaluated using eddy covariance towers at intact and logged sites at the Tapajos National Forest in Brazil and data on long-term dynamics reported in the literature. ED-2 is able to reproduce both the fast (< 5yr) recovery of water, energy fluxes compared to flux tower, and the typical, field-observed, decadal time scales for biomass recovery when no additional logging occurs. The results also indicate that under high-intensity, conventional logging, both the drying near the ground due to canopy opening and the additional fuel loads due to the logging disturbance have the potential to support more intense fires. These results indicate that under intense degradation, forests may greatly increased fire frequency, severely reducing carbon stocks, and inducing long-term changes in forest structure and composition from recurrent fires. The insights obtained from ED-2 shed lights on future directions in representing tropical forest degradation and recovery in similar ecosystem models, such as the Functionally Assembled Terrestrial Ecosystem Simulator (FATES) (See Huang et al., Poster).

Terrestrial Ecosystem Science

Argonne National Laboratory
TES Science Focus Area

Poster #1-32

Determining Soil Organic Matter Composition and Decomposability across the Permafrost Region Using Mid-infrared Spectroscopy

Roser Matamala[1*], Julie Jastrow[1], Francisco Calderon[2], Scott Hofmann[1], and Umakant Mishra[1]

[1]Argonne National Laboratory, Argonne, IL
[2] Central Plains Resources Management Research, USDA. Akron, CO

Contact: matamala@anl.gov

BER Program: TES
Project: TES-SFA ANL
Project Website: http://tessfa.evs.anl.gov/

Soil organic matter (SOM) turnover and stability are largely controlled by environmental and biological factors; however, the chemistry of SOM can also be an important influence on decomposition and soil respiration. In permafrost regions, organic matter is often preserved in a relatively undecomposed and uncomplexed state, both in surface horizons and in buried forms such as peat deposits and cryoturbated organic matter. Because of the large amounts of SOM stored in these soils and differences in the relative importance of SOM stabilization mechanisms operating in the permafrost region compared to other soil types, the composition and potential decomposability of SOM are key uncertainties in models assessing the amount of carbon that might be released from this region. We have demonstrated that mid-infrared (MIR) spectroscopy can provide valuable information to characterize the chemical composition of permafrost-region SOM and its potential decomposability. MIR spectra can be related to many soil attributes including carbon and nitrogen concentrations, land cover type, parent material, pH, and other chemical and physical properties. Furthermore, MIR is very sensitive to the degradation state of SOM, and it is a good predictor of the short-term carbon mineralization potential of tundra soils. We are applying MIR spectroscopy techniques to soils collected by numerous investigators in Alaska, Canada, Greenland, and Russia to create a Soil-IR library of MIR spectra that will enable widespread estimates of SOM composition and potential decomposability across the permafrost region. Using the Soil-IR library, we investigated multivariate relationships between soil properties and MIR spectra that have yielded robust calibrations. We are now exploring the applicability of these calibrations to numerous other archived samples. We have also studied SOM stability indicators of SOM decomposition and maturity using MIR organic functional groups and mineral signature ratios across gradients of climate, vegetation type, and other soil- forming factors. The ultimate goal of our research is to link estimates of SOM composition and potential decomposability with geo-referenced data characterizing soil properties and environmental conditions to create geospatial assessments and maps, which can serve as benchmarks for models at landscape, regional, and global scales.

Poster #1-33

Degradation State of Soil Organic Matter in Arctic Coastal Plain Ice-Wedge Polygons

Julie Jastrow[1*], Roser Matamala[1], Chien-Lu Ping[2], Timothy Vugteveen[1], Jeremy Lederhouse[1], Scott Hofmann[1], Gary Michaelson[2] and Umakant Mishra[1]

[1]Argonne National Laboratory, Argonne, IL
[2]University of Alaska Fairbanks, Palmer, AK

Contact: jdjastrow@anl.gov

BER Program: TES
Project: Argonne National Laboratory SFA
Project Website: http://tessfa.evs.anl.gov/

Estimates of the amount of soil organic matter (SOM) stored in permafrost-region soils and its susceptibility to mineralization or mobilization with changing climate or physical disturbance are improving but remain highly uncertain. In lowland permafrost soils, much of the SOM exists in a poorly degraded state and is often weakly associated with soil minerals due to the cold, wet environment and cryoturbation. Thus, the impacts of permafrost thaw likely will depend, at least initially, on the extent of SOM degradation before incorporation into permafrost. We are investigating particle size fractionation as an indicator of the relative degradation state of SOM in permafrost region soils. Soil samples with bulk soil organic carbon concentrations ranging from 0.8% to 47% (n = 150) and representative of soil horizons in flat-, low-, and high-centered ice-wedge polygons near Barrow, Alaska, were size-fractionated to isolate fibric (coarse; >250 µm) from more degraded (fine; 53−250 µm) particulate organic matter and to separate mineral-associated organic matter into silt- and clay-sized fractions. Data from these samples were used to develop calibration models that can predict the amount of carbon associated with each size fraction from the mid-infrared (MIR) spectra of unfractionated bulk soils. The MIR calibration models were then used to supplement measured data to estimate the size distribution of SOM throughout entire soil profiles (to a depth of 3 m) of the sampled ice-wedge polygons. We found that the relative degradation state of SOM varied spatially and vertically within polygons and differed among polygon types. Our findings suggest that accounting for polygon- related variations could improve estimates of the relative degradation state of SOM in areas dominated by ice-wedge polygons and provide valuable data on the potential decomposability of permafrost region SOM stocks for benchmarking local, regional, and earth system models.

Poster #1-34

Spatial Heterogeneity and Environmental Controllers of Permafrost SOC Stocks

Umakant Mishra[1*], Julie Jastrow[1], Roser Matamala[1], and the Permafrost Carbon Network

[1]Argonne National Laboratory, Argonne, IL

Contact: umishra@anl.gov
BER Program: TES
Project: Argonne National Laboratory SFA
Project Website: http://tessfa.evs.anl.gov/

Permafrost affected soils are a key component of the global carbon cycle and play an important role in moderating the global climate system. Previous permafrost soil organic carbon (SOC) stock estimates used a variety of upscaling approaches and reported substantial uncertainties in the estimates. In this study, we used spatially referenced data of soil-forming factors (topographic attributes, land cover types, climate, and bedrock geology) and pedon description data ($n = 2552$) in a regression kriging framework to predict the spatial and vertical heterogeneity of SOC stocks across the northern circumpolar and Tibetan permafrost regions. This approach allowed us to take into account both the correlation between SOC and environmental factors and the spatial autocorrelation among SOC observations to make separate estimates of SOC stocks and their spatial uncertainties (90% CI) for three depth intervals at 250 m spatial resolution. In the northern circumpolar region, we estimated 510 (449 – 572), 355 (324 – 401), and 298 (255 – 348) Pg C for 0 – 1, 1 – 2, and 2 – 3 m depth intervals, respectively. In the Tibetan region, our estimates were 11 (9 – 13), 3 (0.5 – 6), and 3 (1.4 – 5) Pg C at 0 – 1, 1 – 2, and 2 – 3 m depth intervals, respectively. We captured large spatial variability (coefficient of variation = 13 – 129%) depending upon the study region and depth interval. We found the greatest uncertainty range at 1 – 2 m depth in both permafrost regions. Soil wetness index and elevation were significant controllers of SOC stocks in both regions. Surface air temperature and bedrock geology were significant controllers of permafrost SOC in the circumpolar region, whereas precipitation was a significant controller in the Tibetan region. Flat areas (<2% slope angle) stored the greatest amount of SOC in the northern circumpolar region, but hill toe-slope positions stored the largest SOC stocks in the Tibetan region. In the circumpolar region, the greatest topographic uncertainty in SOC stocks (27%) was in hill toe-slope positions. In the Tibetan region, however, the uncertainty was highest (62%) in flat areas. We believe our results provide the first global assessment of permafrost SOC stocks that is based on quantitative relationships with environmental factors at a high spatial resolution (250-m). We hope our spatially explicit estimates of SOC stocks can be useful for initializing and benchmarking the representation of SOC stocks in regional and global land surface models.

Terrestrial Ecosystem Science

Oak Ridge National Laboratory
TES Science Focus Area

Poster #1-35

ORNL's Terrestrial Ecosystem Science – Scientific Focus Area (TES SFA): A 2018 Overview

Paul J. Hanson[1*], Daniel M. Ricciuto[1] and TES SFA Participants

[1]Environmental Sciences Division, Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

Contact: hansonpj@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: http://tes-sfa.ornl.gov/ and http://mnspruce.ornl.gov/

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:

Improve 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 environmental 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 CO_2 and other greenhouse gases?
3. What are the climate-induced shifts in terrestrial hydrologic and ecosystem processes that inform assessment of climate change impacts on ecosystem services and society?

The ongoing 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 CO_2 on the C feedbacks from a black spruce–*Sphagnum* ecosystem. New SPRUCE results in 2018 include a comprehensive analysis of the C cycle and root production in peatlands, a full evaluation of *Sphagnum* gross primary production, a new publication on the negative response of lichens to warming environments, publications regarding the improvement of peatland ecosystems models, and a number of collaborator publications on bog biogeochemistry. The Fine Root Ecology Database (FRED) has begun to generate published commentaries, and Version 2.0 will be released early in 2018. Work at the Missouri Ozark eddy flux site has advanced our understanding of temperate forest responses to drought and data that were collected from ORNL-designed instrumentation on solar-induced chlorophyll fluorescence used to evaluate OCO-2 advanced photosynthesis observation from space. The TES SFA aims to integrate experimental and observational studies with model building, parameter estimation, and evaluation to yield reliable model projections from site to global scales. New modeling results in 2018 include new methods to estimate model parameter sensitivities and calibration with observations.

Poster #1-36

Impacts of Elevated CO_2 and Whole Ecosystem Warming on Photosynthesis and Respiration of Two Ericaceous Shrubs in a Northern Peatland

Eric J Ward[1*], Jeffrey M Warren[1], Stan D Wullschleger[1], Anthony W King[1], Daniel M Riccuito[1] and Paul J Hanson[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: wardej@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: http://mnspruce.ornl.gov/

The Spruce and Peatland Responses Under Changing Environments (SPRUCE) project is a large-scale, long-term experiment investigating the effects of warming and elevated CO_2 on an 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) CO_2 concentrations for 10 years. This poster focuses on the responses of the two dominant ericaceous shrubs (*Rhododendron groenlandicum* and *Chamaedaphne calyculata*), quantifying the seasonal patterns of photosynthesis and respiration to the first two years of temperature and CO_2 treatments. These two species dominate the understory at this site (~80% of biomass) and are 35% more productive than the trees in this open canopy forest. Whole ecosystem warming extended the physiologically-active season in both spring and fall for these years, increasing the period of active carbon assimilation. Gas-exchange results from the first year exhibited some photosynthetic acclimation to CO_2 treatments and respiratory acclimation to temperature, although the degree of acclimation was species-specific in each case. Nitrogen per unit leaf mass of *R. groenlandicum* decreased under elevated CO_2, but nitrogen per unit leaf area was maintained by a concurrent increase in leaf mass per area. Detailed gas exchange measurements from the second growing season revealed the trade-off between photosynthetic and respiratory rates that underpin a broad thermal optimum of net assimilation rates. We illustrate how these results will be incorporated into modeling efforts for northern peatlands in global dynamic vegetation models.

Poster #1-37

Divergent Morphological and Hydrological Responses of Dominant Woody Bog Species to Whole Ecosystem Warming and Elevated CO_2 at SPRUCE

Jeffrey Warren[1*], Eric Ward[1], Joanne Childs[1], Anirban Guha[1], and Paul J. Hanson[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN

Contact: warrenjm@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: http://mnspruce.ornl.gov/

The SPRUCE climate change experiment has been exposing a southern boreal forested bog to whole ecosystem warming since 2016 and elevated CO_2 (eCO_2) concentrations since 2017.
This long-term project was designed to test mechanistic responses of a vulnerable ecosystem to changing environment conditions in order to inform and improve prognostic terrestrial biosphere models. Using large open-topped chambers, the ecosystem was subjected to increased temperature (T) up to +9 °C that has accelerated spring phenology in the warmest plots by up to 6 weeks. Together with T-driven increases in nutrient availability and vapor pressure deficit, we hypothesize that the treatments would induce changes in morphology and relationships with plant water relations of dominant woody plants. In 2017 we collected terminal shoots that fully developed under treatments from black spruce (*Picea mariana*) (current and year-old cohorts developed under T treatments, but only current cohort under CO_2 treatments), leatherleaf (*Chamaedaphne calyculata*), tamarack (*Larix laricina*), and bog Labrador tea (*Rhododendron groenlandicum*). Morphological plant traits measured included growth rate, leaf mass per area (LMA), branch silhouette to projected leaf area ratio (SPAR), C:N and xylem hydraulic anatomy. Sapflow and predawn/midday water potentials were measured to assess treatment x morphology impacts on plant water relations. In August 2017, LMA declined with T in L. laricina exposed to eCO_2 but increased for aCO_2. In contrast, LMA declined with T in P. mariana under both CO2 treatments (R2=0.63). Whole shoot SPAR values declined with T for *L. laricina* by up to 14%, but increased with T for *P. mariana* by 8% for both CO_2 treatments. In contrast, the *R. groenlandicum* shrub STAR values exhibited a threshold response, declining with T up to +6.75 °C, but increasing dramatically for +9 °C treatments, regardless of CO_2 treatment. We expect there are species-specific limits to foliar plasticity in response to T that may result in ecological advantages those species with broader acclimation capacity. In addition, the divergent responses of the trees may reflect their different anisohydric (*Larix*) or isohydric (*Picea*) strategies. Indeed, in response to T, *P. mariana* closed stomata prior to the *pretreatment* turgor loss point, which maintained water potentials and sapflow at constant levels. In contrast, *L. laricina* kept stomata open in response to T, approaching or exceeding the turgor loss point, dramatically increasing predawn/midday water potential stress and doubling plant water use. Results improve mechanistic understanding of plant responses to future environmental conditions, including net primary productivity, water use and biogeochemical cycling.

Poster #1-38

Sphagnum Production, Nutrient Content, and Community Composition in the SPRUCE Experiment

Richard J. Norby[1*] and Joanne Childs[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN

Contact: rjn@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: http://mnspruce.ornl.gov

Sphagnum contributes a substantial fraction of the net primary productivity of the S-1 bog, and it is the source of the accumulation of peat in the ecosystem. Hence, characterizing *Sphagnum* production and its response to the warming and CO_2 treatments are important objectives of the SPRUCE experiment. We will test the hypothesis that by accelerating soil nutrient cycles, warming will promote shrub production to the detriment of the *Sphagnum* community via increased competition for light and nutrients. We also hypothesize that moss species that are more adapted to drier condition (*Sphagnum magellanicum* and *Polytrichum* sp.), which are present primarily on hummocks, will increase in importance relative to *S. angustifolium* and *S. fallax*. We measured the production and composition of *Sphagnum* community in 10 enclosures and two open plots in 2017. There were five levels of heating (+0 ∘C to +9 ∘C) combined with ambient or elevated (+500 ppm) CO_2. *Sphagnum* productivity was measured by placing a known quantity of either *S. magellanicum* or *S. angustifolium/fallax* (which are difficult to distinguish) in a 3.8-cm diameter mesh tube and inserting the tube in the bog, ensuring close contact with the surrounding *Sphagnum* community. The tubes were installed in October and removed one year later, dry weight of new tissue measured, and the capitula were analyzed for N and P content. Species composition of the moss layer was measured in 25 5×5 cm locations distributed along three transects in each plot. Mosses covered 97% of the ground area of the open plots: 67.6% was covered with *S. angustifolium/falla*x, 20.6% with *S. magellanicum*, and 8.8% with *Polytrichum*. The fraction of area without live moss (bare ground, dead moss, or grass) increased sharply with enclosure temperature, and only 40% of the ground was moss covered in the +9 ∘C enclosures. The fraction of *S. angustifolium*/fallax in the moss-covered area increased with temperature and *S. magellanicum* and *Polytrichum* declined, in opposition to the response we had hypothesized. Sphagnum production in the open plots averaged 440 g m^{-2}. Production of S. *angustifolium/fallax* in both hummocks and hollows declined with increasing temperature; there was no effect of CO_2. Plot-level production was significantly greater in open plots and declined dramatically with increasing temperature in the enclosures. Nitrogen and phosphorus concentrations in *Sphagnum* capitula increased with warming, consistent with evidence of their increased availability. The nitrogen:phosphorus ratio of 9 suggests the *Sphagnum* community is N limited.

Poster #1-39

Insights into Sphagnum Peat Moss Carbon and Nitrogen Dynamics from CO_2 Flux Analysis and Modeling to Microbiome Analysis

David Weston[1*], Alyssa Carrell[2], Anthony Walker[1], Richard Norby[1], Lianhong Gu[1], Joanne Childs[1], Joel Kostka[3], Max Kolton[3], Jana Phillips[1], and Paul J. Hanson[1]

[1]Environmental Sciences Division & Climate Change Science Institute, Oak Ridge National Laboratory
[2]Biosciences Division and Climate Change Science Institute, Oak Ridge National Laboratory
[3]School of Biology, Georgia Institute of Technology, Atlanta, GA

Contact: westondj@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: https://mnspruce.ornl.gov/

Sphagnum mosses are foundation species for many peatland ecosystems. With rapid rates of climate change occurring in high latitudes, vast reservoirs of carbon accumulated over millennia in peatland ecosystems are potentially vulnerable to rising temperature and changing precipitation. We explored the carbon and nitrogen cycling responses of *Sphagnum* to warming and CO_2 enrichment as part of the Spruce and Peatland Responses Under Changing Environments (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) CO_2 within 12-m diameter, open-top enclosures. Peat moss community analysis shows that the SPRUCE site is dominated by *Sphagnum angustifolium*, *S. fallax* (together comprising 68% cover), and *S. magellanicum* (21% cover). Using clear-topped automatic CO_2 chambers, we investigate the seasonal drivers of *Sphagnum* gross primary production (GPP)—the entry point of carbon into wetland ecosystems. Our CO_2 flux analysis and partitioning show that Sphagnum GPP peaked in late summer, well after the peak in photosynthetically active radiation. Wavelet analysis showed that water table height was the key driver of weekly variation in *Sphagnum* GPP in the early summer and that temperature was the primary driver of GPP in the late summer and autumn. We used this information to augment a process-based photosynthetic model that is currently being used by the SPRUCE team. Based on an average *Sphagnum* C:N ratio of 44.3, less than 10% of the N needed to support the observed *Sphagnum* production was accounted for in deposition. Therefore, we explored the impact of SPRUCE imposed experimental warming on the microbial and nitrogen-fixing (diazotroph) community associated with *Sphagnum*. To quantify changes in abundance, diversity, and community composition of *Sphagnum* microbiomes in response to warming, we performed qPCR and Illumina sequencing of SSU rRNA and nitrogenase (*nifH*) genes. Microbial diversity decreased with warming ($p<0.05$), and diazotrophs shifted from diverse communities to domination by *Nostocaceae* (from 25% in unheated samples to 99% in warmed samples), suggesting that warming influences diversity. Furthermore, temperature increase was negatively correlated with N_2 fixation showing that warming in our system resulted in decreased N_2 fixation. Thus, experimental warming may alter the community structure and function of peat moss microbiomes.

Poster #1-40

Warming Increases Plant-Available Nutrients in the SPRUCE Bog

Colleen M. Iversen[1*], John Latimer[2], Deanne J. Brice[1], Joanne Childs[1], Holly M. Vander Stel[1]; Natalie A. Griffiths[1], Avni Malhotra[1], Richard J. Norby[1], Keith Olehieser[2], Steve Sebestyen[3], Eric Ward[1], Jeffrey Warren[1], and Paul J. Hanson[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]XCEL Engineering, Oak Ridge, TN
[3]Center for Research on Ecosystem Change, Northern Research Station, USDA Forest Service, Grand Rapids, MN

Contact: iversencm@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: https://mnspruce.ornl.gov/

Peatlands store nearly one-third of global soil carbon in deep deposits of peat that are shielded from decomposition by acidic conditions, waterlogged soils, and cold temperatures. Warming is expected to increase the release of carbon from highly-organic peatland soils, potentially leading to a positive feedback to future warming. This response is expected to be mediated by the response of peatland vegetation to rising atmospheric [CO_2], as well as the effects of warming on plant-available nutrients and water.

We quantified the effects of a range of ecosystem warming (from +0 °C to +9 °C), as well as elevated [CO_2], on plant-available nutrients in the SPRUCE (Spruce and Peatland Responses Under Changing Environments) experiment in an ombrotrophic bog in northern Minnesota, USA. We used ion-exchange resin capsules to monitor monthly changes in plant-available nutrients (i.e., NH_4-N, NO_3-N, and PO_4^{3-}) throughout the peat profile and across hummock-hollow microtopography. NH_4-N was by far the most available N source, with NO_3^-N making up a negligible fraction; PO_4^{3-} availability was intermediate. After the first full year of increases in temperature and [CO_2], warming—combined with a longer frost-free period—tripled the availability of NH_4^+ and PO_4^{3-} in the warmest treatment plots. However, the increase in nutrients was much greater below the rooting zone. There is thus far no effect of elevated [CO_2] on nutrient availability.

Interestingly, the same warming response was not apparent in the subset of porewater nutrients collected and measured at bi-weekly intervals at a comparable depth increment in the hollows. While porewater total organic carbon concentrations were increased by warming, indicating increased mineralization of organic matter, there was no difference in porewater NH_4^+ NO_3^-, or PO_4^{3-} concentrations across the warmed plots.

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

Poster #1-41

Modeling Nitrogen and Phosphorus Cycling Dynamics and the Interactions with Carbon Cycling in Peatland Ecosystems

Xiaojuan Yang[1*], Dan Ricciuto[1], Xiaoying Shi[1], Paul J. Hanson[1], Colleen Iversen[1], Rich Norby[1], Natalie Griffiths[1], Peter Thornton[1], David Weston[1], Steve Sebestyen[2], Terri Jicha[3], Kirsten Hofmockel[4], Avni Malhotra[1], Joanne Childs[1], Randy Kolka[2], and Scott Bridgham[5]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge, TN
[2]USDA Forest Service, Northern Research Station, Grand Rapids, MN
[3]USEPA Environmental Effects Research Laboratory, Duluth, MN
[4]Environmental Molecular Sciences Laboratory, Richland, WA
[5]University of Oregon, Eugene, OR

Contact: yangx2@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA

Although only covering 2-3% of land's surface, peatland ecosystems store about one third of global soil carbon(C) and are currently considered as sinks for atmospheric CO_2. It is crucial to have a predictive understanding of how this C-rich ecosystem responds to changes in temperature and atmospheric CO_2. One of the key characteristics of peatland ecosystems is the low input of nutrients such as nitrogen (N) and phosphorus (P), particularly in bogs that receive all of their nutrients from precipitation. Primary production in peatlands has been found to be limited by N availability or P availability, or co-limited by both N and P. Despite the important role of N and P in controlling productivity and ecosystem function, limited attention has been paid to investigating the N and P cycling dynamics and how they affect C cycling in peatland ecosystems, particularly in the context of environmental changes. A recent focus of SPRUCE (Spruce and Peatland Responses Under Changing Environments) has been on nutrient cycle, in particular N and P. Comprehensive measurements of major N and P reservoirs and related processes have been conducted for both pre-treatment condition and with treatment. Here we try to integrate these empirical data with a modeling approach aiming to develop a predictive understanding of N and P cycling in peatland bogs in response to environmental changes and how the responses affect C cycling. We use the ELMv1- SPRUCE, which is developed based on the most recent ELM v1 and ELM v0-SPRUCE. Compared to ELMv0-SPRUCE, ELMv1- SPRUCE includes an improved representation of nitrogen cycle and a prognostic phosphorus cycle. The questions we are trying to address include: (1) can the model reproduce the N and P budget from the field measurements; (2) what processes in the model needs to be improved (either process representation or parameterization) or added based on the measurements; (3) what other measurements are needed to better inform model representation; and (4) How do the model simulated responses to warming and elevated CO_2 differ from the experiment and why? The ultimate goal of this study is to improve the representation of N and P cycling processes and C-N-P interactions in ELM-SPRUCE, while the modeling efforts can also help guide the most-needed measurements in the field.

Poster #1-42

Sensitivity of Simulated Peatland Carbon and Energy Flux Warming Responses to Biogeochemistry Process Uncertainty

Daniel Ricciuto[1], Dan Lu[1], Jiafu Mao[1], Xiaoying Shi[1], Anthony King[1], and Paul J. Hanson[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge, TN

Contact: ricciutodm@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA

Uncertainty about land surface processes contributes to a large spread in model predictions about the magnitude and timing of climate change within the 21st century. Land surface models incorporate a diverse array of processes across various temporal and spatial scales, and include dozens of uncertain parameters. As components of complex Earth system models, such as the Energy Exascale Earth System Model (E3SM), these land-surface models provide crucial information about fluxes of water, energy, and greenhouse gases to the atmosphere and oceans. However, the signs and magnitudes of these fluxes depend on multiple competing feedbacks, and model projections diverge in the latter half of this century. Much of the current understanding about land-surface process uncertainties at regional to global scales derives from model intercomparison projects. However, such MIPs conflate structural and parametric uncertainty, so that combining models or drawing conclusions is difficult. Improved understanding about the sensitivity of model outputs to specific parameters and processes, and the contribution of parametric uncertainty to overall prediction uncertainty, is of critical importance for directing future model development and measurements, and for increasing the accuracy of future projections. One method to quantify model parameter uncertainty is global sensitivity analysis (GSA). A large number of GSA methods exist, and different approaches are selected depending on the computational demands of the model simulation, the dimensionality of the problem, and the desired accuracy of the result.

Here we perform a GSA for a peatland version of the E3SM land model (ELM-SPRUCE) at the SPRUCE experiment site. We analyze the sensitivity of hydrologic cycling, soil C cycling, and the growth of multiple plant functional types response to moderate (+4.5 °C) and high (+9 °C) warming scenarios. We find that the model is especially sensitive to autotrophic and photosynthesis temperature response functions, including parameters related to acclimation. To the degree that this parametric uncertainty can be reduced by observations, we can constrain predictions of responses to warming. This uncertainty is then compared to initial simulations from the SPRUCE model intercomparison, providing additional constraints on model structural uncertainty.

Poster #1-43

Initial Effects of Warming and Elevated CO_2 on Organic-Matter Decomposition in a Black Spruce-*Sphagnum* Bog

Natalie A. Griffiths[1*], Randy K. Kolka[2], Colleen M. Iversen[1], Scott D. Tiegs[3], and Deanne J. Brice[1]

[1]Climate Change Science Institute and Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]USDA Forest Service, Northern Research Station, Grand Rapids, MN
[3]Department of Biological Sciences, Oakland University, Rochester, MI

Contact: griffithsna@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: https://mnspruce.ornl.gov/

Peatlands are disproportionately important for landscape carbon storage. These ecosystems store ~30% of terrestrial carbon, primarily in peat, despite comprising only ~3% of global land area. Peat accumulates when primary production exceeds decomposition. Therefore, it is important to understand how decomposition rates are affected by climate change. We are examining the response of organic-matter decomposition to warming and elevated CO_2 within the Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment. SPRUCE uses ten 12-m diameter enclosures built within a bog in northern Minnesota to increase air and peat temperatures (+0, +2.25, +4.5, +6.75, +9 °C) at ambient and elevated CO_2 (eCO_2) (+500 ppm) for 10 years. A litterbag technique was used to measure decomposition rates of 6 litter types that vary in chemical quality (spruce needles and fine roots, Labrador tea leaves and fine roots, and two *Sphagnum* moss species). The litterbags were deployed in both hummock and hollow microtopographies in the SPRUCE enclosures, and the first series of collections in a decade-long experiment were retrieved at 0, 0.5, and 1 years for measurement of dry mass and chemistry. We predicted that decomposition rates would increase with warming, with little effect of eCO2. We also predicted a stronger response in hollows than hummocks if saturated hollows typically become drier with warming and microbial activity increases. After 1 year, fine-root decomposition rates increased with warming (decomposition coefficients increased from 0.33/y to 0.46/y [+0 to +9°C] for Labrador tea roots and from 0.35/y to 0.45/y for spruce roots). There was no clear difference in hummocks vs hollows and no effect of eCO_2. In contrast to roots, all aboveground litter types did not respond to warming or eCO_2. *Sphagnum magellanicum* decomposed slowest (0.27/y), while the 3 other litter types decomposed at a similar rate (Labrador tea leaves 0.51/y; spruce needles 0.50/y; *Sphagnum angustifolium*/*fallax* 0.45/y). A standardized cotton-strip assay (95% cellulose) was also deployed vertically into the peat to examine seasonal, interannual, and depth-specific decomposition rates. In general, tensile loss increased with warming across all depths, suggesting that labile carbon decomposition responds positively to warming. The lack of response of aboveground litter decomposition to warming may be due to differences in chemistry (e.g., labile cotton strips vs less-labile litter) or differences in techniques (e.g., experiment duration). Litter decomposition and cotton strip tensile loss will continue to be measured over the 10-year duration of SPRUCE to understand longer-term decomposition responses to warming and eCO_2.

Poster #1-44

Parallel Computing for Module-based Computational Experiment: A Case Study of Carbon Decomposition using ELM Modules

Dali Wang[1*], Cindy Yao[2], and Daniel Riccuito[1]

[1]Environmental Science Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]The University of Tennessee, Knoxville, TN

Contact: wangd@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA

Many large-scale scientific applications play an important role in improving and exploring our daily life. However, it is often very expensive to maintain those codes, and even more difficult to quantify and evaluate on specific function's effect due to the lower-level program construction and the codes' complexity. Based on previous work on functional unit testing, we developed a data driven parallel computing framework to facilitate module-based computational experiment. By adopting parallel data-driven pipeline and fast IO network, our model achieved a good performance on ORNL's leadership computing facilities. In this research, we extracted key functions from the E3SM land model (ELM) that represent the carbon decomposition process. Then, we compared the performance of the de-composition reaction network within the ELM using data collected from the long-term intersite decomposition experiment team (LIDET). The decomposition submodel is the convergent trophic cascade (CTC) used in a number of studies in the Community Land Model. Since CTC was evaluated using LIDET data previously, therefore, in this study, we first verified that in the LIDET study using our standalone module does not introduce unrealistic feedbacks between the simulated litter bags and vegetation growth. Then we used the standalone CTC submodel to investigate (1) the impacts of default settings of litter decomposition parameters, and (2) the influence of nitrogen limitation, and the temporal variability of its limitation, on litter decomposition.

Poster #1-45

Peatland Respiration: A Global Quantitative Review

Avni Malhotra[1*], Benjamin Bond-Lamberty[2], Paul J. Hanson[1], Mercedes Horn[2], and Colleen M. Iversen[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Pacific Northwest National Laboratory, Joint Global Change Research Institute, University of Maryland, College Park, MD

Contact: Malhotraa@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA, PNNL PREMIS-ghg LDRD
Project Website: https://tes-sfa.ornl.gov

Since the last glacial maximum, peatlands have sequestered vast amounts (600 Gt) of carbon (C) globally. This storage capacity and previously stored C are vulnerable to climate change. Warming and drying of northern peatlands, for example, is expected to increase C losses from these systems and further feedback into climate warming. The magnitude and mechanisms of this increased C loss remains unconstrained. Temperature and moisture changes in peatlands are associated with changes in plant community composition. However, the net result of these abiotic and structural changes on peatland ecosystem respiration globally remains unclear. Over the past three decades, peatland carbon cycling has been studied to estimate rates of production, decomposition and C accumulation. Chamber flux measurements are a common method used to estimate inputs and losses of C. Structural (plant community) and abiotic (moisture, temperature and pH) controls on peatland CO_2 flux have also been investigated in disparate studies but have not been compiled to test overarching hypotheses on structure-C function linkages. It is unclear whether hypotheses about structural controls on C fluxes are true for a diversity of peatlands globally. Modeling future changes in peatland C function and its impacts on the global carbon cycle requires a comprehensive quantitative understanding of previously measured ecosystem dynamics.

We will present a quantitative synthesis of all published peatland CO_2 flux data with a focus on structure-function links in these ecosystems. In addition to compiling the first dataset that incorporates all existing chamber CO2 flux data (ecosystem respiration, ER; and net ecosystem exchange, NEE) from peatlands, we will examine the following questions: 1) what is the spatial and temporal variability of *in situ* ER from northern peatlands, 2) what are the major structural and abiotic controls on peatland CO_2 exchange (focus on plant trait link to flux as well as temperature and moisture sensitivity), 3) what are the remaining knowledge gaps regarding ER and CO_2 exchange in northern peatlands, and 4) can lessons learned from northern peatlands be applied to the less-studied tropical peatlands? This review will synthesize existing knowledge on peatland ER globally, provide a conceptual framework and dataset, and highlight knowledge gaps; all necessary steps toward understanding and modeling future peatland C function.

Poster #1-46

Representing Northern Peatland Hydrology and Biogeochemistry with the ELM Land Surface Model

Xiaoying Shi[1*], Daniel M. Ricciuto[1], Peter E. Thornton[1], Paul J. Hanson[1], Xiaofeng Xu[2], Fengming Yuan, Jiafu Mao[1], Jeffrey Warren[1], Richard J. Norby[1], Steve Sebestyen[3], Natalie A. Griffiths[1], David J. Weston[1], and Anthony P. Walker[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Biology Department San Diego State University, San Diego, CA
[3]USDA Forest Service Grand Rapids, MN

Contact: shix@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: http://mnspruce.ornl.gov

Northern peatlands are likely to be important in future carbon cycle-climate feedbacks due to their large carbon pool and vulnerability to hydrological change. A key objective for our effort is to produce an enhanced model capable of being used for accurate simulations of high-carbon wetland hydrologic and carbon cycle responses and for application to plausible future climate conditions. Current models have begun to address microtopographic controls on peatland hydrology, but none have included a prognostic calculation of peatland water table depth for a vegetated wetland, independent of prescribed regional water tables, and have not treated moss as a plant function type. First, we introduce a new configuration of the land model (ELM) of Energy Exascale System Model (E3SM), which includes a fully prognostic water table calculation for a vegetated peatland. Second, we couple our new hydrology treatment with vertically structured soil organic matter pool, and the addition of components from methane biogeochemistry. Third, 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. Next, we use our new model structure to test the how the carbon and water cycles will respond to elevated CO_2 and different warming scenarios.

Poster #1-47

Nonlinear Response of Soil Microbial Respiration to Moisture Variations

Junyi Liang[1*], Shikha Singh[2], Sindhu Jagadamma[2], Daniel M. Ricciuto[1], Lianhong Gu[1], Paul J. Hanson[1], Jeffrey D. Wood[3], Christopher W. Schadt[1], Gangsheng Wang[1], and Melanie A. Mayes[1]

[1]Environmental Sciences Division & Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, Tennessee
[2]Department of Biosystems Engineering and Soil Science, University of Tennessee, Knoxville, Tennessee
[3]School of Natural Resources, University of Missouri, Columbia, Missouri

Contact: liangj@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: https://tes-sfa.ornl.gov/

Globally, soils store over twice as much carbon (C) as the atmosphere. As such, a small change in soil C content may have a large impact on the magnitude of atmospheric CO_2 concentrations, and therefore on climate. Soil microbial respiration, one of the most important CO_2 effluxes from soils to the atmosphere, is dependent on soil moisture conditions. However, the magnitude of microbial respiration in response to drought and wetting is still unclear. Here, we conducted a laboratory incubation experiment and a modeling study to reveal how soil microbial respiration responds to soil moisture variations. In the laboratory incubation experiment, two soils (a sandy soil and a loamy soil) were incubated under a moisture gradient from air dried to complete saturation. The microbial respiration showed a bell-shape response to the moisture variation, with the optimum between 50% and 100% of water holding capacity. In the modeling study, we extended the experimental results by conducting a theoretical analysis of the response of soil microbial respiration to intensified soil moisture extremes by the end of the 21st century at a temperate forest (i.e., MOFLUX site). Results showed that the magnitude of reduced microbial respiration by drought was generally greater than that of increased microbial respiration by wetting, suggesting an asymmetric response of microbial respiration to soil moisture variations. Further analysis indicated that the asymmetric response of microbial respiration was due to greater responses of active microbial biomass and specific respiration rate to drought than to wetting. As a consequence, increased frequency and severity of soil moisture extremes reduced soil C loss through microbial respiration. Both the experimental and modeling studies emphasize the non-linear response of soil microbial response to moisture variations. Currently, most soil carbon studies are focused on temperature responses, while this study points to the importance of the sensitivity of soil CO_2 fluxes to moisture.

Poster #1-48

A System for Long-Term Continuous Solar-Induced Chlorophyll Fluorescence Measurements for Synergy with Eddy Covariance Flux Networks

Lianhong Gu[1], Jeffrey D. Wood[2], Christine Yao-Yun Chang[3], and Ying Sun[3]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]School of Natural Resources, University of Missouri, Columbia, MO
[3]School of Integrative Plant Science, Cornell University, Ithaca, NY

Contact: lianhong-gu@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA

Solar-induced chlorophyll fluorescence (SIF) is a direct probe of canopy photosynthesis that provides critical information on the dynamics of terrestrial gross primary production—a unique role that cannot be achieved using any other method. Therefore, long-term continuous SIF observations have the potential to greatly advance terrestrial ecosystem science and applications. Realizing and exploiting this potential requires synergistic implementation of SIF measurements within eddy covariance (EC) flux networks—the backbone of contemporary ecosystem research—because the two measurements provide independent, but complementary information. We currently lack a robust SIF measurement system that can withstand harsh environmental conditions and integrate seamlessly with instrumentation at flux tower sites. Here, we introduce the Fluorescence Auto-Measurement Equipment (FAME) and protocol that fulfill such a purpose. FAME's innovative hardware and software designs aim at versatility, extensibility, autonomous operation, and ease of maintenance for the acquisition of SIF data of unprecedented quality and quantity. FAME has the unique feature that the same system measures ancillary environmental variables at the precise time of spectral irradiance sampling, allowing for the proper interpretation of SIF signal. The FAME prototype has been deployed since September 2016 at the top of a 32 m walkup tower in an oak-hickory forest at the Missouri Ozark AmeriFlux site, and has provided stable measurements even when air temperatures approached 40 °C. Preliminary results reveal that canopy SIF saturates at high light, similar to leaf-level photosynthesis. Furthermore, clear patterns of diurnal hysteresis were observed whereby for the same light level, morning SIF was higher than in the afternoon. We hypothesize that the dynamics of non-photochemical quenching and movements of chloroplasts and leaves may explain the observed pattern. The technology and measurement protocol introduced here advances the coordinated observation of SIF and EC fluxes, and thus represents a step-change in observational ecosystem and carbon-cycle science.

Poster #1-49

Forest Ecosystem-scale Responses and Resilience to Drought

Jeffrey D. Wood[1*], Christian Frankenberg[2], and Lianhong Gu[3]

[1]University of Missouri, Columbia, MO
[2]California Institute of Technology, Pasadena, CA
[3]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: woodjd@missouri.edu

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: https://tes-sfa.ornl.gov/?q=node/15

The observation and modeling of ecosystem responses to stress are major challenges in carbon (C) cycle science. We examined ecosystem response and resilience during the exceptional 2012 US drought in an oak-hickory forest, synthesizing flux tower, ecophysiological and satellite observations with an ensemble of GPP models. During drought, gross primary productivity (GPP) was suppressed and the ecosystem was a net C source for ~50 days during July and August. Ecosystem function recovered rapidly after soaking rains, such that the forest was a net C sink through the end of the growing season. Data-driven models (MODIS, MPI) and the Community Land Model (CLM) bracketed observations—significantly over- or underestimating drought response and resilience, and in the case of CLM, failing to simulate the early season GPP peak during well-watered conditions. In contrast, solar-induced fluorescence showed excellent coherence with observed GPP, despite a large scale-mismatch between the satellite and ground-based observations, demonstrating site-level skill at tracking GPP and associated dynamics due to plant water stress. Taken together, there is a pressing need for integrated observational and modeling investigations to better characterize and represent ecosystem stress responses in models, with particular emphasis on improving the representation of stomatal conductance.

Poster #1-50

ORNL's TES SFA Data Acquisition, Archiving, and Sharing to Support Publications, Synthesis, and Modeling Tasks

Les A. Hook[1*], Jeffery S. Riggs[2], Misha B. Krassovski[1], W. Robert Nettles[1], Ryan R. Heiderman[3], and Paul J. Hanson[1]

[1]Environmental Sciences, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Logistical Services Divisions, Oak Ridge National Laboratory, Oak Ridge, TN
[3]Michigan Technological University, Houghton, MI

Contact: hookla@ornl.gov

BER Program: TES
Project: ORNL Terrestrial Ecosystem Science SFA
Project Website: https://mnspruce.ornl.gov/ and https://tes-sfa.ornl.gov/

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. What's new and improved for the ORNL TES SFA?

FRED 2.0: Version 2 of the Fine Root Ecology Database (FRED) has been released at https://roots.ornl.gov/. FRED 2.0 contains more than 105,000 observations of some 330 different types of root traits as well as associated data such as site soil temperature, moisture, and sunlight, from about 1,200 data sources. There are more than 1.5 x 10^6 reported values. This is a 50% increase in observations and sources above and beyond FRED 1.0.

Phenocam Expansion at SPRUCE: New closeup shrub-view cameras have been added in each SPRUCE experimental chamber to supplement the existing overhead-view. See https://phenocam.sr.unh.edu/webcam/gallery/.

Gigabit Internet Connection at SPRUCE: High-speed internet connectivity via fiber optics will reach the SPRUCE Site. This new connection will facilitate direct access to data loggers, automated minirhizotron cameras, soil flux chamber instruments, real-time Phenocam images, the eddy covariance (EC) flux system, and a new mobile integrated EC/SIF (solar-induced chlorophyll fluorescence) system.

FAME at MOFLUX: The Fluorescence Auto-Measurement Equipment (FAME) SIF measurement system, has been deployed at the Missouri Ozark AmeriFlux (MOFLUX) site. FAME provides stable measurements over a wide range of conditions. The developing field technology and measurement protocols facilitate coordinated observation of SIF and EC fluxes, that will lead to new advances in ecosystem and carbon-cycle science.

DOIs via OSTI: The TES-SFA can now register DOIs for data products using the OSTI (Office of Scientific and Technical Information) E-Link System. Comprehensive metadata can be entered that will facilitate the eventual transfer of data to the ESS-DIVE archive.

New Data Products: Check for new datasets and modeling products from ORNL SPRUCE and TES SFA Teams plus DOE, EPA, and Universities at our project web sites.

Poster #1-51

The FACE-MDS Dataset

Anthony Walker[1], Tom Boden[1], Andrew Burton[2], Bruce Hungate[3], Lynn Fernstermaker[4], Patrick Megonigal[5], Robert Nowack[6], Ram Oren[7], Elise Pendall[8], Alan Talhelm[9], Bai Yang[10], Donald Zak[11], FACE-MDS team, and Richard Norby[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Michigan Tech, Houghton, MI
[3]Northern Arizona University, Flagstaff, AZ
[4]University of Nevada, Las Vegas, NV
[5]Smithsonian Environmental Research Center, Edgewater, MD
[6]University of Nevada, Reno, NV
[7]Duke University, Raleigh, NC
[8]Western Sydney University, Sydney, New South Wales, Australia
[9]University of Idaho, Moscow, ID
[10]NOAA, Idaho Falls, ID
[11]University of Michigan, Ann Arbor, MI

Contact: walkerap@ornl.gov

BER Program: TES
Project: FACE Model Data Synthesis project
Project Website: https://facedata.ornl.gov/facemds/

Predictive understanding of the future terrestrial carbon sink remains elusive and terrestrial ecosystem responses to increasing CO_2 are a large contributor to uncertainty in this understanding. The FACE Model Data Synthesis (FACE-MDS) project has been working for close to the past 10 years to synthesize data from FACE experiments and an ensemble of terrestrial ecosystem models to help improve our predictive understanding of the future terrestrial carbon sink. In Phase 1 of the FACE-MDS (2008-2012) the FACE experiments at Duke University and Oak Ridge National Laboratory were analyzed. In Phase 2 (2012-2016) three more FACE sites, Rhinelander, Wyoming PHACE, and the Nevada desert FACE, as well as the Florida scrub oak Open Top Chamber experiment were brought into the synthesis. While some of the data (meteorological and model) were made publicly available from Phase 1, the ecosystem response data and Phase 2 data were not. This presentation coincides with the release of the full dataset from the FACE-MDS project. The dataset includes data from all six sites and is broken out into three different datasets: 1) meteorological data; 2) model output data, as well as protocol and site parameterization data; and 3) ecosystem response data. We aim to release the FACE-MDS dataset on the ESS-DIVE by the time of the ESS PI Meeting. This presentation will show some of the key features of the dataset.

Terrestrial Ecosystem Science

Lawrence Berkeley National Laboratory
TES Science Focus Area

Poster #1-62

Berkeley Lab Terrestrial Ecosystem Science SFA (LBNL TES SFA) on Belowground Carbon Cycling

Margaret S. Torn[1*], Eoin Brodie[1], Peter Nico[1], William J. Riley[1], Rose Abramoff[1], Cristina Castanha[1], Katerina Georgiou[1], Rachel C. Porras[1], and Jennifer L. Soong[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: mstorn@lbl.gov

BER Program: TES
Project: LBNL TES SFA

In the Berkeley Lab Terrestrial Ecosystem Science SFA, we conduct basic research on the role of soils in terrestrial biogeochemistry and the Earth system. Our goals are to improve process-level understanding of ecosystem-climate interactions and to develop next-generation predictive capacity suitable for Earth system models. Current research in the SFA is centered around a set of field, laboratory, and model 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 a field manipulation experiment in a well-drained coniferous forest in which we are warming the whole soil profile (+4ºC) and adding ^{13}C-labelled litter at different soil depths. We are using the experiments to evaluate the influence of soil depth, mineralogy, biota, and climate on soil carbon dynamics, and applying the results and observations to inform model structures and parameters. Currently, a small number of groups world-wide are developing models for global-scale application that represent explicitly processes that limit microbial utilization of organic substrates, like sorption to minerals and nutrient limitation. 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. Incubations, and other studies to guide model development in a reactive transport framework (using BeTR; Tang et al. 2013), and integrating this model into a version of the DOE E3SM land model (ELM). This poster will present results from the two warming experiments and highlight some recent results from the microbial and geochemical work being carried out in the SFA. Highlights for the warming experiment and modeling will be given in separate posters.

Poster #1-63

Four Years of Warming the Whole Soil Profile in a Conifer Forest: LBNL TES SFA

Jennifer Soong[1*], Rose Abramoff[1], Katerina Georgiou[1], Cristina Castanha[1], Rachel C. Porras[1], and Margaret S Torn[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: jsoong@lbl.gov

BER Program: TES
Project: LBNL TES SFA

Soils contain three times as much carbon as the Earth's atmosphere, with approximately half of the total soil carbon stocks in subsoil horizons. The storage of carbon as soil organic carbon, and its exchange with the atmosphere through decomposition, is critical to the maintenance of Earth's climate. However, the impact of warming on decomposition throughout the whole soil profile is a major source of uncertainty in climate projections. Here, we present the results from four years of the first *in situ*, replicated, whole soil warming experiment. The experiment is located at the University of California Blodgett Experimental Forest in a mixed coniferous forest in the foothills of the Sierra Nevada mountains in California at 1370 m above sea level. Three replicate pairs of 3 m in diameter, warmed and un-warmed plots were constructed in 2013 and heating began in October 2014. Vertical heating cables maintain a +4°C warming above the ambient plots temperatures down to 1 m depth. Soil surface fluxes have been measured monthly and total annual soil respiration is 34-37% greater in warmed plots than control plots with an average monthly Q_{10} temperature response of 2.4. Monthly sampling of CO_2 concentrations throughout the soil profile, along with soil profile diffusion flux modeling, reveals that soil CO_2 production in the deep soil increased by a similar amount. Sampling of soil pore water using lysimeters at 20 and 70 cm shows a significant increase in total organic carbon concentrations in the warmed plots at both depths. Together, the results from soil CO_2 flux measurements and soil pore water sampling indicate greater decomposition of soil organic carbon under 4°C warming and a similar degree of vulnerability of deep soil and surface soil organic carbon to loss. Warming of the whole soil profile reveals a much larger response than currently predicted by other in situ soil warming experiments that only warm the soil profile and thus fail to account for the impact of soil warming on deep soil carbon losses.

Poster #1-64

LBNL TES SFA Development and Application of Explicit Biotic and Abiotic Models for Soil Organic Matter Dynamics

William J. Riley[1*], Rose A. Abramoff[1], Katerina Georgiou[1], Jinyun Tang[1], and Margaret S. Torn[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: wjriley@lbl.gov

BER Program: TES
Project: LBNL TES SFA

In the LBNL TES SFA we are developing land model components to improve understanding, analyses, and predictive capability of the complex, inter-connected processes that affect Soil Organic Matter (SOM) dynamics. This poster describes new approaches to represent soil microbial physiology, substrate use, enzymatic and microbial temperature and moisture sensitivity, and mineral surface and plant interactions. We will describe recent applications of these models to our whole-soil profile warming experiment, long-term fallow observations, and analyses of future SOM dynamics. We are also working to integrate these conceptual advances into the new DOE E3SM land model (ELM) using the integrated BeTR reactive transport solver. Broadly, our results indicate that explicit representations of the aforementioned processes improve prediction of SOC dynamics under multiple simultaneous stressors, thereby providing more realistic scenarios of future C cycle dynamics.

Poster #1-65

Steady State Gradients versus Microbe-Mineral Modeling Predict Different Temperature Responses of Upland Soils: Model Evaluation in the LBNL TES SFA

Rose Z. Abramoff[1*], William J. Riley[1], Katerina Georgiou[1], Jinyun Tang[1], and Margaret S. Torn[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: mstorn@lbl.gov

BER Program: TES
Project: LBNL TES SFA

Modelers and empiricists often use spatial data to characterize soil organic carbon (SOC) stock responses to warming and to test climate predictions in the absence of long-term warming measurements. This “space-for-time” approach assumes that the decadal-scale warming responses of SOC stock are similar to the steady-state relationship between temperature and SOC stocks at spatially distributed sites. This assumption, however, is poorly tested. Using a process- rich soil model, we found that while different ways of representing temperature-response can give equally good predictions of steady-state SOC stocks, the transient response of SOC stocks to warming differs greatly.

We developed four variants of a reaction-network-based model of soil organic matter and microbes (ReSOM) using measured SOC stocks from a large latitudinal transect. Each model featured different assumptions about the temperature sensitivity of microbial activity and mineral sorption. All model versions made similar SOC stock predictions at steady state but predicted transient warming responses that differed in the sign and magnitude of change. We compared these different predictions for SOC stock to the latitudinal dataset and a large metanalysis of observed warming impacts. Models that did well and that did poorly at matching the warming response of SOC stock were indistinguishable when compared to steady state observations; in other words matching the steady state temperature gradient data did not mean that the model could produce consistent or accurate predictions of change under temperature changes. We also found that for the largest SOC pool, the mineral-associated SOC , direct temperature sensitivity was not required to cause large changes in stock due to the connection with DOC. Specifically, even in cases where mineral-SOC (i.e., sorption kinetics) was not directly affected by temperature, the model predicted a large change in SOC stock due to the warming effect on decomposition rates of the aqueous (i.e., desorbed) SOC. Mineral-associated C changed by -0.3 to +0.09 kg C m^{-2} K^{-1} yr^{-1} when only microbial activity is temperature sensitive due to interactions between the mineral-surface and the dissolved monomer C that is vulnerable to microbial consumption. In conclusion, steady state and “space-for-time” observations may be inadequate for constraining or evaluating a models’ ability to predict the response of soil carbon cycling to rapid environmental change. Both microbial and mineral mechanisms affect these dynamics.

Terrestrial Ecosystem Science

Pacific Northwest National Laboratory
Soil Biogeochemistry Study

Poster #1-57

Drought and Flood Alter Soil Pore Connectivities and Local Ionic Strengths to Regulate C Bioavailability

Vanessa Bailey[1*], Peyton Smith[1], Taniya Roy Chowdhury[2], Sarah Fansler[1], Kathe Todd-Brown[1], Lisa Bramer[1], and Ben Bond-Lamberty[3]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]University of Maryland, College Park, MD
[3]Joint Global Change Research Institute, Pacific Northwest National Laboratory, College Park, MD

Contact: vanessa.bailey@pnnl.gov

BER Program: TES
Project: PNNL Project

The extent and duration of extreme moisture events such as inundation and drought are projected to increase as climate continues to change globally. As soils are alternatively in dry or wet conditions, water, or the lack of it, drives the soil carbon cycle across a wide range of spatial scales. Quantitative elucidation of these processes is needed to evaluate the degree of uncertainty that can be mitigated by including this knowledge in next generation land-carbon models.

Hydrologic connection within the soil pore network is a determinant of the transport potential of both SOC species and of any planktonic soil microorganisms. It couples with ionic strength in that the local ionic strength is a factor controlling the relative desorption of complex versus simple SOC species. It is unknown, however, how this affects the potential transport or mobilization of microorganisms.

The objective of this research was to evaluate the combined role of water as a solvent and as a conduit on soil C cycling, by measuring the effect of drought vs saturation on the mobilization of soil C in three different soils exposed to laboratory manipulations. Three hypotheses are addressed: i) soils subjected to a simulated drought will have greater proportions of complex C species in their pore waters; ii) soils subjected to extended saturation will have a greater proportion of simpler C; and iii) soils held at field-moist conditions will reflect the resource islands that occur as a result of discontinuous water connections and have the greatest chemical diversity. We found that inundation events following drought can significantly increase the quantity of C in soil pore waters compared with soils that were previously field-moist. Even when the *quantity* of soluble C in pore waters is unchanged by historical drought, the *quality* of the C in the soluble pool changes. This suggests that the chemical and biological processes that occur in response to extreme hydrologic events are sensitive to soil and ecosystem moisture history.

Poster #1-58

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

Ben Bond-Lamberty, [1*] and Vanessa Bailey[2]

[1]Joint Global Change Research Institute, Pacific Northwest National Laboratory, College Park, MD
[2]Pacific Northwest National Laboratory, Richland, WA

Contact: bondlamberty@pnnl.gov

BER Program: TES
Project: PNNL Project

Soil carbon (C) persistence in soils is unpredictable in the face of extreme wetting and drying as its protection mechanisms are not understood well enough to incorporate into process-rich simulation models. While much research has focused on the size of the soil organic C (SOC) pool and its gross fluxes, new approaches in SOC characterization and modeling can now address the very nature of SOC persistence, specifically the contributions of physical occlusion and chemical composition to C longevity.

Despite the importance of soil structure and hydrology for SOC protection and destabilization, Earth system models remain grounded in structures in which first-order transfers among SOC pools are proportional to the size of the donor pool. Such models are based on C “quality,” an ill- defined term that cannot be measured directly and cannot represent rewetting dynamics such as the respiration response to water movement through pores and the role of water as a solvent within pores. Finally, scale point measurements of decomposition and greenhouse fluxes to tower or landscape/watershed scales, a critical requirement for effective use of such data in ESMs, remains highly uncertain.

Our objective is to develop the process-rich understanding of how SOC is decomposed as a result of pore-scale changes in SOC physical protection under varying antecedent moisture conditions, and use this knowledge to improve the predictive power of models at a variety of scales.

Terrestrial Ecosystem Science

Lawrence Berkeley National Laboratory
AmeriFlux Management Project

Poster #1-69

Updates from the AmeriFlux Management Project Tech Team

Sébastien C. Biraud[1*], Stephen Chan[1], Sigrid Dengel[1], Dave Billesbach[2], Chad Hanson[3], Pascal Polonik[1], and Margaret S. Torn[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]University of Nebraska, Lincoln, Lincoln, NE
[3]Oregon State University, Corvallis, OR

Contact: scbiraud@lbl.gov

BER Program: TES
Project: AmeriFlux Management Project
Project Website: https://ameriflux.lbl.gov

AmeriFlux is a network of more than 250 sites where ecosystem CO_2, water, and energy fluxes are measured by the eddy covariance method. AmeriFlux is also a network of the tower PIs and thousands of scientists who use the data, to study terrestrial ecosystems and quantify their role in global environmental change. The AmeriFlux Management Project (AMP) Data Team serves the network with technical support (the subject of this poster), data support, outreach, and maintaining a set of long-term sites.

The AmeriFlux Management Program (AMP) Tech Team at LBNL strengthens the AmeriFlux Network by (1) standardizing operational practices, (2) developing calibration and maintenance routines, (3) setting clear data quality goals, and (4) assessing instruments and new tools. In this poster we will present results and recent progress in four areas:

- Sonic anemometers firmware problem in commonly used Gill Sonic anemometers.
- Unmanned aerial systems (UAS), and sensors systematically used at AmeriFlux sites to improve site characterization.
- IRGA intercomparison for flux measurements (LI-COR, Picarro, and Campbell Scientific), see also poster by Polonik et al.
- New calibration services and lessons learned during site visits

Poster #1-70

Side-by-side Evaluation of Eddy Covariance Gas Analyzers for the AmeriFlux Network: Effects of Analyzer Type and Spectral Corrections on Turbulent Fluxes

P. Polonik[1*], W.S. Chan[1], S. Dengel[1], D.P. Billesbach[2], G. Burba[3], J. Li, A. Nottrott[4], I. Bogoev[5], B. Conrad[5], and S.C. Biraud[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]University of Nebraska, Lincoln, Lincoln, NE
[3]LI-COR Biosciences Inc., Lincoln, NE
[4]Picarro Inc., Santa Clara, CA
[5]Campbell Scientific Inc., Logan UT

Contact: ppolonik@lbl.gov

BER Program: TES
Project: AmeriFlux Management Project
Project Website: https://ameriflux.lbl.gov

The eddy covariance (EC) technique is used at hundreds of field sites worldwide to measure trace gas exchange between the surface and the atmosphere. Data quality and correction methods for EC have been studied empirically and theoretically. Recent development of new gas analyzers for CO_2 and H_2Ohas led to an increase in options for EC practitioners. Gas analyzers can be categorized based on their sample and inlet configuration as open-path, closed-path, or enclosed-path sensors. We evaluated the comparability of fluxes calculated from five different gas analyzers including two open-path (LI-7500A, IRGASON), two enclosed-path (EC200, LI-7200), and one closed-path (Picarro) analyzers, which were all located on a single tower in an irrigated alfalfa field managed by University of California, Davis. To effectively compare sensors with different inlet characteristics, the use of corrections to account for signal loss was required. Therefore, we applied two spectral corrections (Massman and Fratini methods) and a purely empirical approach using the integrals of sensible heat and gas cospectra. We found that all fluxes calculated from the gas analyzers were comparable if appropriately corrected. However, the comparability strongly depended on the gas species (CO_2 or H_2O) and the correction method chosen. Differences were below 5% on average for CO_2 fluxes using any correction method, but for H_2O, the average differences were between 4% and 13% for the different correction methods. The magnitude of corrections also varied strongly, especially for water vapor fluxes. This study does not identify a best sensor, but considers the benefits and difficulties of each sensor and sensor type. This information should be considered by investigators when choosing a sensor for a site or when analyzing EC measurements from multiple sites.

Poster #1-71

AmeriFlux Data Processing and Interface Improvements

Danielle Christianson[1*], Housen Chu[2], You-Wei Cheah[1], Gilberto Pastorello[1], Yeongshnn Ong[1], Fianna O'Brien[1], Dario Papale[3], Marty Humphrey[4], Deb Agarwal[1], and Margaret S Torn[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]University of California, Berkeley, Berkeley, CA
[3]University of Tuscia, Viterbo, Italy
[4]University of Virginia, Charlottesville, VA

Contact: dschristianson@lbl.gov

BER Program: TES
Project: AmeriFlux Management Project
Project Website: https://ameriflux.lbl.gov

The AmeriFlux Management Project (AMP) Data Team offers a wide array of services to the flux tower teams and data users including: an archive, QA/QC processing, DOIs, and standardization of flux and meteorological data. In this poster, we introduce recent advances that are described below.

The AmeriFlux Data Team QA/QC data-processing pipeline accepts data in the new standardized half-hourly flux data submission format (called FP-In). Automated QA/QC checks are performed and results are communicated with flux-tower teams via on-line reports and a customized issue tracking system. After successfully passing the QA/QC assessment, the data is published in the FP-Standard half-hourly format. This standardization allows automation of the data processing which has resulted in rapid turn-around of processing and feedback to data submitters. In addition, the standard format significantly expands the number and types of variables included in the data submissions and data products. Over 50 sites have successfully submitted data in FP-In format, and the data are available on the AmeriFlux website. Flux-tower teams can track their site's data processing status via a new page on the AmeriFlux website. The AmeriFlux QA/QC assessment incorporates many of the checks that were developed in the production of the major synthesis data release, FLUXNET2015. The FP-Standard data output from the AmeriFlux QA/QC data processing will be ready for gap-filling, partitioning, and the next generation of FLUXNET processing. For more information on the data standards and services, see ameriflux.lbl.gov and ameriflux.lbl.gov/data/aboutdata/data-variables/.

The Biological, Ancillary, Biological, and Metadata (BADM) templates, used to organize and share non-flux data from tower sites, continue to evolve. The BADM web submission and update interface allows tower teams to easily provide incremental data submissions and corrections of the site general information BADM data (ameriflux.lbl.gov/data/badm-data-templates/). We have updated the vegetation cover and soil BADM templates and are testing new interface formats to improve the ease of collecting and submitting BADM data. In addition, we developed a new web tool for submitting height and instrument model information for flux-met data. This tool also maps historical data formats to the new FP-In format. The data team is continually working to improve the flux-tower PI and user experience in 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 #1-72

The Data Processing Pipelines and Synthesis Dataset Releases for AmeriFlux and FLUXNET

Gilberto Z. Pastorello[1*], Danielle S. Christianson[1], Housen Chu[2], You-Wei Cheah[1], Abdelrahman A. Elbashandy[1], Carlo Trotta[3], Eleonora Canfora[3], Dario Papale[3], Dennis Baldocchi[2], Deb A. Agarwal[1], and Margaret S. Torn[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]University of California, Berkeley, Berkeley, CA
[3]University of Tuscia, Viterbo, Italy

Contact: gzpastorello@lbl.gov

BER Program: TES
Project: AmeriFlux Management Project
Project Website: https://ameriflux.lbl.gov

The new AmeriFlux BASE flux-data product and the FLUXNET2015 dataset, which includes data from 86 AmeriFlux sites, are being used extensively by the scientific community. We have seen a growing interest in these datasets, with increasing number of users registering with the AmeriFlux and FLUXNET web sites to be able to access the data. This trend also shows on the number of downloads of site data. This poster will show usage statistics for data products available directly at the AmeriFlux portal and as part of the FLUXNET2015 dataset. We will also describe the data-processing pipelines generating these data products, highlighting improvements in data quality control processes, decreased processing time, additional derived data products, and new coding efforts that are continuously making software more robust to execute. These improvements enable updates to these data products more consistently and in a timelier manner. The next iteration for the FLUXNET global datasets is scheduled for release in the summer of 2019, and we will be using these improved tools in our data-processing pipelines. We will make these software tools available to the community so that site teams and data users can run the same pipelines and reproduce processing results.

Poster #1-73

Developing New Partitioning Methods for AmeriFlux, to Detect and Account for the Inhibition of Day-Time Ecosystem Respiration

Trevor F. Keenan[1*], Mirco Migliavacca[2], Dario Papale[3], Dennis Baldocchi[4], Margaret S. Torn[1], and Thomas Wutzler[2]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Max Planck Institute for Biogeochemistry, Jena, Germany
[3]University of Tuscia, Viterbo, Italy
[4]University of California, Berkeley, Berkeley, CA

Contact: trevorkeenan@lbl.gov

BER Program: TES
Project: AmeriFlux Management Project
Project Website: https://ameriflux.lbl.gov

The global land surface absorbs about a third of anthropogenic emissions each year, due to the difference between two key processes: ecosystem photosynthesis and respiration. Despite the importance of these two processes, direct observations of either are lacking. Eddy-covariance (EC) measurements are widely used as the closest 'quasi-direct' ecosystem-scale observation from which to estimate ecosystem photosynthesis and respiration. Recent research, however, suggests that current partitioning methods may be biased by up to 25%, due to a previously unaccounted-for process: the inhibition of leaf respiration in light. Yet the extent of inhibition at the ecosystem scale remains debated, and impacts on global estimates of photosynthesis and respiration unquantified. Here, we quantify the extent of inhibition of ecosystem respiration across both AmeriFlux and the global FLUXNET EC network, and identify a pervasive influence that varies by season and ecosystem type. We develop new partitioning methods that account for inhibition, and find that diurnal patterns of ecosystem respiration might be markedly different than previously thought. The methods developed will be used to produce the next generation of data products from AmeriFlux and FLUXNET.

Subsurface Biogeochemical Research

Lawrence Berkeley National Laboratory
SBR Science Focus Area

Poster #21-71

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

Susan Hubbard[1*], Kenneth H. Williams[1], Deb Agarwal[1], Jillian F. Banfield[2], Harry Beller[1], Nicholas Bouskill[1], Eoin Brodie[1], Reed Maxwell[3], Peter Nico[1], Carl Steefel[1], Heidi Steltzer[4,5], Tetsu Tokunaga[1], Haruko Wainwright[1], and the Watershed Function SFA Team

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]University of California, Berkeley, CA
[3]Colorado School of Mines, Golden, CO
[4]Rocky Mountain Biological Laboratory, Gothic, CO
[5]Fort Lewis College, Durango, CO

Contact: sshubbard@lbl.gov

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

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 a predictive understanding of watershed-scale hydrological and biogeochemical functioning is challenging, as complex interactions occurring within a heterogeneous landscape 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 remains high.

The Watershed Function project aims to substantially reduce this uncertainty through developing a predictive understanding of how mountainous watersheds retain and release water, nutrients, carbon, and metals to downstream users and stakeholders. In particular, the project is exploring impacts of early snowmelt, drought, and other disturbances on mountainous watershed dynamics over seasonal to decadal timescales. The Watershed Function project is being carried out in a headwater catchment of the Upper Colorado River Basin – the East River watershed, which has rapidly evolved into a ‘community watershed’. This site is characterized by significant gradients in elevation, vegetation and hydrogeology. A system-of-systems 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 archetypal subsystems, each having distinct vegetation-subsurface biogeochemical-hydrological characteristics.

We are acquiring and using diverse observations and newly developed models to explore bedrock-to-canopy and terrestrial-to-aquatic interactions and exhanges across this site. The work uses a combination of intensive and satellite sites than span the watershed, with an intial focus on the response to early snowmelt along a lower montane hillslope-to-floodplain transect, as well as exploring the aggregated watershed response to the perturbation. A key technological goal is the development of scale-adaptive simulation capabilities capable of incorporating genomic and other small-scale information where and when it is useful for predicting the aggregated watershed response to disturbance.

Through developing and integrating new microbial ecology, geochemical, hydrological, ecohydrological, computational and geophysical approaches, the project is developing cutting edge approaches to study complex watershed processes and hydrobiogeochemical dynamics spanning genome to watershed scales. This poster will describe project and site and will highlight some of the key recent advances associate with the watershed project.

Poster #21-72

Hillslope to Watershed Subsurface Hydrologic and Biogeochemical Exchanges with the Atmosphere and River

Tetsu Tokunaga[1*], Bhavna Arora[1], Jiamin Wan[1], Adi Lavy[2], Erica Siirila-Woodburn[1], Boris Faybishenko[1], A. Phuong Tran[1], Wendy Brown[3], Joseph Rungee[4], Markus Bill[1], John Christensen[1], Mark Conrad[1], Jillian F. Banfield[2], and Kenneth H. Williams[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]University of California, Berkeley, Berkeley, CA
[3]Rocky Mountain Biological Laboratory, Gothic, CO
[4]University of California, Merced, Merced, CA

Contact: tktokunaga@lbl.gov

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

Studies focused on a lower montane hillslope draining into the East River, Colorado are providing insights into depth-distributed subsurface water flow and biogeochemical transformations, and their coupling to the atmosphere and river. Surface and subsurface measurements of aqueous and gas phase compositions, pressures, and temperatures are being obtained within a 200 m long transect sampled down to 10 m below the soil surface at four stations. Hydraulic potential measurements show seasonally dependent recharge and evapotranspiration influences within the upper 2 m, underlain by baseflow through the fractured Mancos Shale.

Understanding of mountainous watershed subsurface cycling of C and other elements is emerging through quantifying depth-, location-, and season-resolved inventories and fluxes of carbon and nutrients, including OC, IC, C/N, $\delta^{13}C$, ^{14}C, SOM speciation, isotopic analyses as well as respiration rates from laboratory-simulated field conditions. Soil to bedrock chemical composition and mineralogy reveal weathering fronts and weathering contributions to C and metals cycling. Microbially-mediated biogeochemical processes impact large-scale exports from the watershed. Genome resolved metagenomes coupled with metatranscriptomes allow exploration into how the microbial community interacts with these cycles and are employed to study the metabolism of microbial communities at three subsystems within the watershed: the hillslope transect, meander- associated floodplain, and grassland hillslopes.

22-year simulations of evapotranspiration using semi-analytical formulas and the Community Land Model indicate that 55% of the watershed averaged annual precipitation is lost due to evapotranspiration, and 75% of which occurs from May to September. Partitioning of ET indicates that transpiration, soil evaporation, and canopy evaporation account for ~50%, 32%, and 18% of total ET. ET is greater at the middle elevation of ~3000 m, where both air temperature and LAI are largest, and smaller along the river valley and at high elevations. Primary controls on water, carbon, and nitrogen fluxes along the hillslope are being investigated with 2-D (x-z) models. An integrated groundwater-surface water model of the East River basin is being used to obtain upper boundary conditions for the models. Historical meteorological data are being used to simulate representative wet and dry years with early and late snowpack melt, to understand impacts of antecedent conditions during extreme weather years. Simulation results indicate significant heterogeneity in hydrologic and biogeochemical fluxes. Water and nitrogen fluxes are higher around footslope regions following snowmelt. Analyses of geochemical data indicate the importance of dilution from snowmelt infiltration in upslope regions and the prominence of iron and nitrate reduction in footslopes.

Poster #21-73

Vegetation and Soil Biogeochemistry Feedbacks as Impacted by Snowmelt Regime and Landscape Topography

Eoin Brodie[1*], Bhavna Arora[1], Elizabeth Ballor[2], Harry R. Beller[1], Markus Bill[1], Nicholas J. Bouskill[1], Romy Chakraborty[1], Mark Conrad[1], Baptiste Dafflon[1], Brian Enquist[1], Nicola Falco[1], Amanda Henderson[3], Ulas Karaoz[1], Alex Polussa[1], Patrick O. Sorensen[1], Heidi Steltzer[2,4], Haruko Wainwright[1], Shi Wang[1], Kenneth H. Williams[1], Chelsea Wilmer[2,4], and Yuxin Wu[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Rocky Mountain Biological Laboratory, Gothic, CO
[3]University of Arizona, Tucson, AZ
[4]Fort Lewis College, Durango, CO

Contact: elbrodie@lbl.gov

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

In recent years, decreasing snowpack and early snowmelt have been observed with increasing frequency in the mountainous west. Changes in the hydrologic cycle, particularly early snowmelt or reduced snowpack are hypothesized to disrupt coupled plant-microbial behavior, possibly due to the temporal discontinuity between microbial nutrient release and vegetation greening around the snowmelt period. The objective of this work is to determine the mechanisms underlying feedbacks between hydrologic and biogeochemical fluxes, microbial metabolism and vegetation phenology/physiology. We particularly focus on comparing these process couplings for an average hydrologic year (e.g., 2016) to variations due to a deep snow pack (as observed in 2017) or an unusually sparse and early melting snowpack (as observed in 2018).

Remote sensing and machine learning using training data from lower montane ecosystem hillslope transects was employed to classify vegetation and to quantify distributions of functional types (shrubs, forbs, grass) and multiple representatives of these functional groups were selected for simulations using the *ecosys* land-atmosphere model. Autonomous *in situ* measurements of seasonal temperature and water availability through the soil and subsurface demonstrated contrasting insulating effects of snow cover on soil temperature regimes and feedbacks between surface soil temperature and soil water movement under snow, with consequences for nitrogen retention following snowmelt. *Ecosys* simulation results demonstrate distinct spatial signatures of hydrological and biogeochemical fluxes along the hillslope transect, with greater evapotranspiration rates and higher soil water storage in the floodplain as compared to upslope regions. Consistent with observations, simulated water and nitrogen fluxes are higher around the backslope region following snowmelt. Model simulations indicate that nitrogen runoff after snowmelt impacts vegetation community structure, resulting in islands of fertility around the backslope. Soil depth, and topographic features such as slope and curvature are currently being investigated as key factors defining vegetation distributions and phenology.

Ecosys simulations also show that an earlier, and larger, soil water nitrate concentration occurs with advanced snowmelt due to atmospheric warming and that differences in snowpack depth alterthe under-snow nutrient buffer, particularly ammonium concentrations. In both scenarios of simulated early snowmelt and decreased snowpack, slrrub dominance was observed at the site. These results clearly indicate a temporal connection between snowmelt-associated nutrient release and shrubification at the hillslope site.

Poster #21-74

Perturbing Nature: Will a Small Change in the Timing of Snowmelt Lead to Big Shifts in Soil-Plants-Microbes and Watershed Behavior?

Heidi Steltzer[1,2*], Patrick Sorensen[3], Chelsea Wilmer[1], Eoin Brodie[3], Harry Beller[3], Markus Bill[3], Nicholas Bouskill[3], Romy Chakaraborty[3], Mark Conrad[3], Brian Enquist[4], Nicola Falco[3], Amanda Henderson[4], Ulas Karaoz[3], Lorah Patterson[4], Alex Polussa[3], Shi Wang[3], Haruko Wainright[3], Ken Williams[3], Xiaoqin Wu[3], and Yuxin Wu[3]

[1]Rocky Mountain Biological Laboratory, Gothic, CO
[2]Fort Lewis College, Durango, CO
[3]Lawrence Berkeley National Laboratory, Berkeley, CA
[4]University of Arizona, Tucson, AZ

Contact: dr.heidi.steltzer@gmail.com
B
ER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

In temperate mountain watersheds, snowmelt is a major hydrologic event associated with large annual fluxes of nitrogen among soils-plants-microbes, as well as a major driver of nitrogen export from watersheds. Plant phenology has historically been triggered by loss of winter snow and air temperature in spring. Plant production and nutrient uptake occurs after snowmelt and is coupled with microbial biomass turnover and soil nutrient mobilization. The coupling likely enhances ecosystem nitrogen retention; however, rising winter and spring air temperatures, dust- on-snow, and reduced winter snowfall is causing snowmelt to take place earlier with increasing frequency in the mountainous western U.S. We hypothesize that early snowmelt will disrupt coupled plant-microbial behavior, resulting in temporal asynchrony between microbial biomass turnover, nutrient release, and the timing of plant leaf expansion. Therefore, a subtle shift in the timing of plant growth due to earlier snowmelt could substantially affect watershed behavior.

Winter 2017 was typical of winters past in the Colorado Rocky Mountains with high snowfall and late-lying snow into June and July. Lower elevations in the East River watershed began greening in mid-May, approaching 100% species with leaves expanded in early June. Drought conditions followed, so that full leaf color change for the early-greening species began in mid- June at lower elevations. Synchrony in greening across a hillslope was greater at lower than higher elevations, where snow cover is more spatially variable. Also, due to high snowfall in 2017, elevations above 11,000 feet began greening nearly three weeks after lower and mid elevation regions of the watershed. This threshold behavior across elevation in the watershed may be a critical watershed behavior that shifts in years with earlier snowmelt. In 2017, at lower elevations, overwinter soil microbial biomass production was triggered by snowmelt infiltration, which occurred more than 60 days prior to soils becoming snow-free. Soil bacterial and fungal community composition, determined by amplicon-sequencing, exhibited striking shifts in the abundance and distributions of taxa and functional guilds. Changes in soil bacterial and fungal community structure was initiated by snowmelt infiltration and persisted through the complete loss of snow in spring. Immediately following snowmelt, NO_3^- concentrations in soil pore water and soil extracts increased dramatically, suggesting release of nitrogen from microbial biomass. These data provide an incredible baseline to compare to this year, 2018, and subsequent years, in which there is a high probability of lower snowfall, earlier snowmelt, and in which earlier snowmelt experiments will take place.

Poster #21-75

Integrated Imaging of Above and Below Ground Properties and their Interactions

Nicola Falco[1*], Baptiste Dafflon[1], A. Phuong Tran[1], Haruko Wainwright[1], Yuxin Wu[1], Emmanuel Leger[1], John Peterson[1], Zhao Hao[1], Chelsea Wilmer[2], Heidi Steltzer[2], Roelof Versteeg[3], Eoin Brodie[1], Kenneth H. Williams[1], and Susan Hubbard[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Fort Lewis College, Durango, CO
[3]Subsurface Insights, Hanover, NH

Contact: NicolaFalco@lbl.gov

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

Watershed systems are characterized by extreme hydrological and pedological heterogeneity that directly impacts the local biotic activity, making plant communities extremely heterogeneous. The ability to characterize such heterogeneity and quantify its coupling with topographic and soil properties is extremely important to predict watershed functioning and responses to hydrological perturbations, such as droughts, floods, and early snowmelt.

In this study, we exploit advanced geophysical and remote sensing (RS) techniques to improve the identification and the understanding of interactions between plant community distribution and dynamic and subsurface properties at various spatial and temporal scales. Data fusion and analysis is complemented by data-constrained, process-based simulation of the influence of soil, vegetation and geomorphic characteristic on hydrological fluxes. This framework is applied in the East River watershed in Colorado, which is a representative Upper Colorado Basin headwaters catchment. We evaluate linkages between physical properties, metrics extracted from digital elevation models and vegetation spectral signature using airborne datasets and multiple ground- and drone-based surveys. We perform our investigation during the growing season in a 500 by 500 m hillslope-floodplain subsystem of the watershed.

First, the data integration shows that geomorphological and soil property spatial variations exert a strong influence on plant community distribution. Second, the temporal variability in the relationship between plant vigor and soil electrical conductivity indicates the significant control of early spring soil condition on plant growth. Further, the ingestion of such diverse data into a process-based data-model assimilation framework enables improvements in the estimation of the hydraulic parameters as well as hydrological and thermal fluxes (incl., evapotranspiration, infiltration). The estimated flux responses indicate how short duration snowmelt events exert a significant influence on water recharge in vadose zone and aquifer. Moreover, the comparison between data and process-based simulation reveals significant potential for improving the estimation of fluxes and their feedback within and between vegetation distribution and soil properties.

Overall, results show that integration of RS data with geophysical measurements provides an unprecedented window into critical zone interactions, revealing significant below- and above-ground co-dynamics. Ongoing research is focusing on the estimation of plant biogeochemical and soil physical and geochemical properties from plant spectral signatures, and an approach to transfer information about the landscape organization and connectivity obtained from RS to larger scales. The developed approaches as well as those currently under investigation are expected to greatly improve our ability to constrain multi-scale, multi-physics hydro-biogeochemical simulations of mountainous watershed responses to hydrological perturbations.

Poster #21-76

Spatial and Temporal Dynamics of Nitrogen in a Mountainous Watershed

Nicholas J. Bouskill[1*], Taylor Maavara[1], Bhavna Arora[1], Markus Bill[1], Eoin Brodie[1], Mark Conrad[1], Benjamin Gilbert[1], Michelle Newcomer[1], Patrick Sorensen[1], Carl Steefel[1], and Kenneth H. Williams[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: njbouskill@lbl.gov

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

Mountainous watersheds are characterized by substantial heterogeneity in geomorphology, soil texture, and vegetation that determine hydrological flow paths and residence times through catchment subsystems. Despite advances in understanding the spatial and temporal drivers of biogeochemical cycling within snowmelt-dominated ecosystems, knowledge gaps remain. Here we describe ongoing work employing a combination of field and laboratory approaches alongside multi-scale modeling to characterize and quantify the sources, transformations, and sinks of nitrogen, a major limiting nutrient, within the East River (CO) watershed. This work focuses on two spatial scales, a hillslope to floodplain transect, and across the whole watershed. At the hillslope scale, we employ a combination of geochemistry, isotope geochemistry and molecular microbiology to identify and quantify specific mechanisms regulating the input (e.g., nitrogen fixation, Mancos shale weathering, atmospheric deposition), retention (plant and microbial accumulation), transformation (mineralization, nitrification) and loss (denitrification or hydrological export) of nitrogen across temporal aridity gradients (capturing baseflow, snowmelt, drought, and monsoonal precipitation). At the watershed-scale we use an auto- calibrated, semi-distributed mechanistic model to ask the question of how broad features of the landscape (e.g., topography, land cover type, soil properties) and biology determine the export of nitrogen (as $NO3^-$ or organic nitrogen) throughout the water year. Our model output is benchmarked against high-resolution nitrate and organic nitrogen flux data collected along the East River and major tributaries over 3+ years. Overall, this work intends to improve understanding of the feedback between climate change-driven hydrological perturbations (in the formation and loss of snowpack) and biogeochemical processes to improve predictions of nitrogen export at the watershed scale.

Poster #21-77

Floodplain Processes Impacting Water Quality and Nutrient and Metal Export

Patricia Fox[1*], Michelle Newcomer[1*], Dipankar Dwivedi[1], Wenming Dong[1], Nicholas J. Bouskill[1], Markus Bill[1], Mark Conrad[1], John Christensen[1], Christian Dewey[2], and Peter Nico[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Stanford University, Stanford, CA

Contact: psnico@lbl.gov

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

The advances derive from a combined effort of field observation, laboratory experimentation, and integrative modeling focused on assessing how biogeochemical processes in floodplain soils and sediments impact the release of carbon, nutrients, and metals to the river. In order to measure the effect of spring snowmelt (a major annual hydrologic forcing event in the system) on nutrient and metal release from sediments we installed a transect of depth-resolved piezometers across Meander C, parallel to an existing transect of piezometers. Water was collected from both transects from peak river discharge (June 2017) through the falling limb (October 2017) at high temporal resolution (every 3-7 days). Strong temporal trends correlated to river stage were observed for DOC and dissolved Fe as well as other nutrient and metal species. In some locations, strong correlations between Fe and trace contaminants (e.g., As) were also observed, emphasizing the link between redox processes and contaminant release. In addition, we tracked elemental concentrations and isotopic compositions of surface and subsurface water and gas through punch probe sampling at key stages of the hydrograph. These data were more spatially extensive than the piezometer data, being collected at multiple locations across the floodplain and stream bed hyporheic zone. In addition, we instrumented a 2nd floodplain site (Meander Z) to allow for future comparisons with the Meander C location. To complement the field efforts, laboratory batch incubation experiments were conducted with sediment from selected depths from Meander C transects under site-specific redox conditions. Results revealed that DOC plays a key role in metal mobility significantly enhancing Fe(II) solubility through the formation of DOC-Fe(II) complexes which dominate Fe(II) aqueous speciation. Field and laboratory data were used to constrain two distinct but complementary modeling efforts, a vertical streambed hyporheic zone model that included microbial and flow feedback dynamics as well as a lateral cross-meander 2D reactive transport model. The stream bed hyporheic zone model suggested that the hyporheic zone can serve many roles throughout the year, as a net source and sink for nutrients, and that the dynamics are strongly forced by the size of the snowpack. The cross meander simulations indicate that low water conditions following high water conditions caused subsurface exports of inorganic and organic carbon, nitrogen, and iron to increase up to 91%, 63%, 75%, and 61%, respectively, further emphasizing the important role of transient hydrologic conditions on floodplain and hyporheic zone biogeochemical processes.

Poster #21-78

Meander-Associated Riparian Zone and Hillslope Floodplain Sites Share Similar Microbial Community Structure and Metabolic Potential

Adi Lavy[1,2*], Paula B. Matheus[1], Wenming Dong[2], Brian C. Thomas[1], Kenneth H. Williams[2], Tetsu Tokunaga[2], Jiamin Wan[2], Susan Hubbard[2], and Jillian F. Banfield[1,2,3]

[1]Department of Earth and Planetary Sciences, University of California, Berkeley, CA
[2]Lawrence Berkeley National Laboratory, Berkeley, CA
[3]Department of Environmental Science, Policy and Management, University of California, Berkeley, CA

Contact: adilavy@berkeley.edu

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

Watershed functioning relies on complex interactions among vegetation, hydrology, topography, and geology. These interactions differ in distinct subsystems of the watershed, such as river floodplains, alpine meadows, and grassland hillslopes. Microbial-mediated biogeochemical processes that occur at the micron-scale in these subsystems impact the large-scale aggregated export from the watershed, including nutrients, carbon compounds and other elements. The current study focuses on two subsystems of the East River headwaters catchment (Colorado, USA), as part of the Watershed Function SFA led by Lawrence Berkeley National Laboratory. One of the subsystems is a meander-associated floodplain (Meander L; ERML), from where 32 riparian soil samples at the 10-25 cm depth were collected (spanning an area of ~ 10,000 m^2). The second subsystem is a hillslope site (Pump House Lower Montane, PLM4) ~ 360 m southeast of ERML, from which samples were collected at 5-15, 30-40, 60-70, and 90-100 cm (9 samples total). Samples were sequenced at the Joint Genome Institute. Our goal is to use these metagenomic datasets to study the soil microbial communities from each site. The research involves reconstruction of near-complete genomes that are used to determine the extent to which the functions of microbial communities of the two subsystems overlap.

Preliminary results based on profiling of community composition using scaffolds encoding ribosomal protein S3 (rpS3) show overlap between the most abundant members of the microbial communities across sites. Likewise, Bacteria are one to two orders of magnitude higher in abundance than Archaea. Thaumarchaeota, archaea that perform ammonia oxidation, are more abundant than Euryarchaeota. Notably, Candidate Phyla Radiation (CPR) taxa are more abundant in samples taken at the floodplain close to the water table (above and below). These novel bacteria are predicted to be heterotrophs and symbionts of other bacteria. Overall, we have obtained at least 250 near-complete genomes from the two subsystems. In topsoil from the two floodplain sites (hillslope and Meander L) Betaproteobacteria are the most abundant group, and based on near-complete genomes, we predicted that they are involved in sulfur oxidation. Deltaproteobacteria are the second most abundant proteobacteria, and they are predicted to carry out sulfate-reduction. Near complete genomes of Acidobacteria, Bacteroidetes, Chloroflexi, Nitrospirae, Planctomycetes, Venucomicrobia, among others; in addition to candidate phyla (CP) Rokubacteria and Latescibacteria (WS3X), and members of the candidate phyla radiation (CPR) such as Parcubacteria and Microgenomates were obtained from both sites. In-depth analysis of the metabolic potential at each site is underway.

Poster #21-79

Nutrient and Metal Release from Shale Weathering Processes Occurring Across Multiple Scales

Allison Sharrar[1*], Sirine Fakra[2], Sergio Carrero Romero[1,2], Xiaoqin Wu[2], John Christensen[2], Romy Chakraborty[2], Jillian F. Banfield[1], and Benjamin Gilbert[2]

[1]University of California, Berkeley, CA
[2]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: asharrar@berkeley.edu

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

Shale weathering releases harmful elements and nutrients into watershed ecosystems. It is driven by rock–water reactions typically influenced by microbial processes. As climate change alters precipitation patterns, a mechanistic understanding of weathering pathways is essential for anticipating impacts on watershed ecosystems. To study this process, soil and a bedrock core were collected from a shale hillslope within the East River watershed of Colorado. Weathering rinds along bedrock fractures were analyzed with synchrotron μXRF and μXANES spectroscopy. In addition, XRD and bulk geochemical measurements via ICP-MS and ICP-AES were made throughout the hillslope. Weathering profiles at both scales include sharp pyrite reaction fronts and accumulation of redox-sensitive elements at redox boundaries, indicating that these elements might not be released into the watershed. The carbonate reaction fronts at the hillslope and fracture scales are offset from the pyrite oxidation profiles. There is evidence of re- precipitation of carbonate and pyrite at the fracture and hillslope scales, respectively. We infer that fundamental weathering reactions are overprinted by changing redox conditions driven by the seasonally fluctuating water table. In another experiment, lab incubations of shale from the site with East River water showed a slow release of sulfate up to 2mM. Towards the end of the three-month incubation, organic carbon and ammonium were also released as a result of shale weathering.

Poster #21-80

Quantifying Magnitude and Age of Groundwater Flux from Topographically Complex Watersheds Using a MODEX Approach

Rosemary Carroll[1*], Kenneth Williams[2], Zhufeng Fang[1], Andrew Manning[3], Reed Maxwell[4], Erica Woodburn[2], Markus Bill[2], and Mark Conrad[2]

[1]Desert Research Institute, Reno, NV
[2]Lawrence Berkeley National Laboratory, Berkeley, CA
[3]U.S. Geological Survey, Lakewood, CO
[4]Colorado School of Mines, Golden, CO

Contact: Rosemary.Carroll@dri.edu

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

The magnitude and age of groundwater contributions to watershed outflows in snow-dominated, mountainous watersheds are poorly understood due to difficulty in characterizing complex surface and subsurface geospatial characteristics and their tight coupling with recharge and associated groundwater connectivity. We explore the hypothesis that deeper, older groundwater is hydrologically active in headwater basins underlain by fractured shale and igneous bedrock through a modeling-experimental (MODEX) framework. Specifically, we highlight three individual studies that can inform one another and update the conceptual model of groundwater flux in these systems. All three studies are conducted within the East River, a headwater basin of the Colorado River and the study site of Berkeley Lab's Watershed Function Science Focus Area (SFA). The first study investigates the lag of snowmelt to stream discharge combining observed mass flux of $\delta^{18}O$ with numerically simulated hydrologic boundary fluxes and inverse techniques applied to analytically-derived transient travel time distributions. Results indicate that snowmelt during wet years transports a greater fraction of younger water (< 1 year) to streams but simultaneously activates older and potentially deeper groundwater contributions in comparison to dry years. The second study combines measurements of multiple dissolved gas tracers (SF_6, CFCs, N_2, and noble gases) and ^3H to constrain age distributions in groundwater samples across key watershed sub-components including shallow and deep groundwater, springs and baseflow. The resulting age information and associated uncertainties are addressed with respect to sampling protocols, excess air and recharge temperature corrections, choice of distribution (e.g. piston flow, exponential, bi-modal), and solution uniqueness. Lastly, a newly developed Lagrangian particle tracking code is applied to an integrated hydrologic model to explore changes in source waters and age distributions of watershed outflows as functions of variable climate. The comparison of results acquired from these three studies provides insight into the age, magnitude, and circulation depth of hydrologically active groundwater in mountainous watersheds and will help guide future observation and modeling strategies performed as part of the SFA project.

Poster #21-81

Spatiotemporal Variability of Ecohydrological Responses to Climate Perturbations in Headwater Watersheds

Haruko Wainwright[1*], Michelle Newcomer[1*], Taylor Maavara[1], Nicholas Bouskill[1], Nicola Falco[1], Rosemary Carroll[2], Kenneth H. Williams[1], and Susan Hubbard[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]Desert Research Institute, Reno, NV

Contact: hmwainwright@lbl.gov

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

Snow-dominated headwater catchments are critical for water resources throughout the world; particularly in the Western US. Under climate change, the temperature increase is known to be amplified in mountainous regions where a large amount of snow is stored. Over the last three decades, there have been many studies reporting changing snowpack conditions and subsequent shifts in plant communities in headwater catchments. However, observational studies are quite limited to quantify how these changes – in temperature, snowpack, and plant communities – affect watershed eco-hydrological responses as well as riverine exports that fuel downstream ecosystems.

This study presents a data-driven multi-scale approach to quantify the effect of exogenous climate drivers on snowmelt, plant phenology, and streamflow dynamics in a headwater watershed, by examining their inter-annual variability and trends over the last 30 years. Motivating our work is the long-term observation of decreasing nitrogen concentrations and fluxes over the past 30 years despite large variability in temperature as well as precipitation and discharge, suggesting a systematic change in watershed scale ecosystem functioning. At the East River, Colorado, where long-term historical changes have been reported, we use a variety of long-term spatially extensive datasets (incl., snow, climate, streamflow, water quality, plant productivity (NDVI), elevation, vegetation) to guide hypothesis development. Results indicate that temperature – particularly spring temperature – has a significant control not only on the *timing* of snowmelt, plant NDVI, and peak flow, but also on the *magnitude* of peak NDVI, peak flow, annual discharge, and river nutrient concentrations. High correlation among June temperature, peak NDVI and annual discharge suggests that spring evapotranspiration limits streamflow volume. Nitrogen and Carbon fluxes, when assessed along the upstream to downstream flow-path, show scaling behavior with watershed characteristics such as drainage area and peak flow. Our results indicate that this observed scaling behavior is affected by the antecedent winter dry or wet conditions of the watershed as a whole. In headwater watersheds above 8,000ft elevation, our yearly flux data show a significant correlation with the average yearly watershed scale NDVI, indicating a biogeochemical link between climate, vegetative response, and watershed exports. Our data-driven approach provides powerful tools that enable the linkage between watershed behaviors of importance such as total flow and nutrient exports to predict future watershed responses to climate change.

Poster #21-82

Watershed Function Simulation and Aggregation

Carl I. Steefel[1*], Reed Maxwell[2], Sergi Molins[1], Dipankar Dwivedi[1], Bhavna Arora[1], Erica Woodburn[1], Zexuan Xu[1], Taylor Maavara[1], Michelle Newcomer[1], Madison Burrus[1], Nicolas Spycher[1], Lauren Foster[2], and Mohammad Danesh[2]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]Colorado School of Mines, Golden, CO

Contact: CISteefel@lbl.gov

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

Watershed hydrological processes mediate a wide range of biogeochemical interactions, ranging from vegetation growth to elemental and nutrient cycling to contaminant fate and transport. However, there are huge uncertainties associated with predicting how watersheds will respond to such perturbations (e.g., droughts or floods) at space and time scales relevant to the management of environmental and energy strategies. In particular, we lack capabilities to predict (1) how watersheds function - that is, how the different parts of a watershed work together to cycle water, nutrients, carbon and other elements - from bedrock to canopy, from across terrestrial and aquatic interfaces, and along environmental gradients; (2) how watersheds respond to atmospheric perturbations, particularly episodic changes in temperature and precipitation; and (3) what watershed properties and processes are critical to include in mechanistic watershed models that feed larger-scale models, such as E3SM or the National Water Model (NWM).

Complementing modeling activities focused on intensive study sites in other components of the Watershed Function SFA, the Watershed Reactor effort aims to understand and predict the aggregated behavior of the system affected by coupled hydrological, energy, and biogeochemical processes. One important challenge is the resolution of hot spots (spatially focused zones of intense hydrological or biogeochemical activity) and hot moments (transient events with potentially outsized impact on system function). As an example, hydrological flow and biogeochemical processes may generate meter scale gradients in concentration in reactive floodplains, and these may need to be captured in models to accurately represent fluxes. Since the overall size of the floodplain system can be quite large, however, efforts are underway to develop scaling motifs based on stream sinuosity, in parallel with similar efforts on hillslopes and deep bedrock that feed water and nutrients to the river system. These upscaling analyses will serve as the basis of a new reactive transport model developed for the Lower Triangle (between the Copper Creek and the PumpHouse). In addition, we use high resolution hydrological modeling based on the ParFlow-CLM software, we have developed an approach to calculating travel time distributions for water within the East River watershed. We will use this in conjunction with a newly developed watershed reactive transport capability combining ParFlow-CLM and CrunchFlow. These residence time distributions, in addition to providing a quantification of the overall water budget within the East River watershed, provide input for distributed, residence time-based models for nitrogen fate and transport.

Poster #21-83

Data Management and Assimilation for the Berkeley Lab Watershed Function SFA

Charuleka Varadharajan[1*], Roelof Versteeg[2], Boris Faybishenko[1], Valarie Hendrix[1], Matthew Henderson[1], and Deb Agarwal[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]Subsurface Insights, Hanover, NH

Contact: cvaradharajan@lbl.gov

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

The Watershed Function SFA project generates heterogeneous datasets at its East River field site that include a variety of data types such as hydrological, geochemical, geophysical, microbiological and remote sensing data. The data are collected from various sources, including data generated by the project team (e.g. sensor data, geochemical sampling and remote sensing products), data from collaborators, and data from external sources (e.g. USGS and NRCS).

The objective of the Data Management and Assimilation (DMA) component of the SFA is to enable science by: (1) managing and archiving the data collected by the project, and releasing those data publicly with appropriate citation information, (2) enabling the project team and the broader community to find where, when and what types of data are being collected through an interactive portal, (3) performing quality assurance and quality control of priority datasets and (4) creating an data integration engine and search portal that can help retrieve, fuse and visualize the diverse data for further synthesis and analysis. The DMA team has developed a number of tools for data management and preservation, QA/QC, data discovery, search and visualization.

Data preservation and distribution are being enabled by a web portal that allows authorized users to upload and download data files as packages. The tool requires users to enter metadata needed to enable web searches and obtain DOIs for citation.

A public interactive map of data collection sites run by the SFA and its collaborators is available at https://wfsfa-data.lbl.gov/watershed/, to inform the broader community about SFA field activities. Sites can be filtered by their key measurements and other metadata, leading to detailed site landing pages.

Automated data QA/QC is performed using statistical methods to identify and flag issues in meteorological, water level and geochemical data. These data are used for example in estimating evapotranspiration estimates or building a set of model drivers (temperature, precipitation, solar radiation, etc.) from the network of meteorological stations, and the river discharge from field observations.

Data integration is achieved via a brokering service BASIN-3D 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.

These tools 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.

Subsurface Biogeochemical Research

Pacific Northwest National Laboratory
SBR Science Focus Area

Poster #21-1

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

Tim Scheibe[1*], Xingyuan Chen[1], James Stegen[1], Maoyi Huang[1], Jie Bao[1], Tim Johnson[1], Hyun-Seob Song[1], Chris Strickland[1], Xuesong Zhang[1], Gautam Bisht[2], Jesus Gomez-Velez[3], Glenn Hammond[4], and Heping Liu[5]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]Lawrence Berkeley National Laboratory, Berkeley, CA
[3]New Mexico Institute of Mining and Technology, Socorro, NM
[4]Sandia National Laboratories, Albuquerque, NM
[5]Washington State University, Pullman, WA

Contact: Tim.Scheibe@pnnl.gov

BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

The PNNL SFA is developing predictive understanding of processes that govern influences of hydrologic exchange flows on water quality, nutrient dynamics, and ecosystem health in dynamic river corridor and watershed systems. Exchange of water between rivers and 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 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 are developing fundamental understanding of i) effects of mixing of pools of organic carbon with different concentration and thermodynamic favorability on biogeochemical reactions (Graham et al. and Song et al. posters); ii) impacts of variable river flows expressed in terms of inundation history on biogeochemical reactions (Song et al. poster); iii) variability of hydrologic exchange processes and carbon biogeochemistry in dynamic river systems across a wide range of geographical settings (Stegen et al. poster); iv) the nature of hydromorphic structure and its impacts on HEFs (Hou et al. and Bao et al. posters); v) integrated impacts of variable river stage and hydrologic exchange at the reach scale (Chen et al. poster); and vi) impacts of HEFs on watershed-scale nutrient processing and water quality (Zhang et al. poster).

SFA research builds on this foundation to develop comprehensive scientific understanding of the influences of HEFs (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 are pursuing the resolution of scientific hypotheses to advance understanding of coupled hydrobiogeochemical processes. At the same time, we are developing 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 human impacts on water quality and riverine ecosystems, and supporting environmentally responsible management of linked energy-water systems.

Poster #21-2

Influence of Hydrologic Exchange Flow on Nutrient Dynamics in Managed Watersheds

Xuesong Zhang[1*], Yilin Fang[1], Xingyuan Chen[1], Maoyi Huang[1], Jesus Gomez-Velez[2], Patrick Royer, Zhuoran Duan, Glenn Hammond, Pin Shuai, Xuehang Song, Hyun-Seob Song, and Tim Scheibe[1]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]New Mexico Institute of Mining and Technology, Socorro, NM
[3]Sandia National Laboratory, Albuquerque, NM

Contact: Xuesong.Zhang@pnnl.gov

BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of PNNL SBR SFA seeks to enhance understanding of the role of hydrologic exchange flow in hydrobiogeochemical cycling at the watershed scale. Hydrologic exchange increases surface water's contact time with reactive environments within the hyporheic zone (HZ), facilitating biogeochemical reactions and influencing fate and transport of solutes along the river corridor. Here, we propose and implement a novel watershed modeling framework by coupling the Soil and Water Assessment Tool (SWAT) watershed model and the PFLOTRAN subsurface reactive transport model, via a new Multi-rate Multi Transfer (MRMT) module. Mass transfer between a river reach and multiple subsurface storage zones within a HZ is modeled with a series of first-order mass transfer coefficients and probability density function (PDF) of coefficients in the limit. Within this framework, we also model a two-step denitrification and oxidative respiration reaction as representative biogeochemical processes within the HZ. This integrated modeling framework allows us to examine dynamics of mass transfer between rivers and HZs along the river corridor within a watershed, and to predict constituent transport and transformation at downstream locations.

As a proof-of-concept, we apply the integrated watershed modeling framework in the Upper Columbia-Priest Rapids watershed to investigate influence of the HZ on watershed nutrient cycling. In this modeling effort, mass transfer rates between river reaches and HZs are derived from the mean residence time as predicted by the hyporheic flow model -- Networks with EXchange and Subsurface Storage (NEXSS). Initial modeling results indicate that irrigation can significantly increase groundwater discharge and nitrate loading into river networks. We design different scenarios to yield quantitative understanding of the role of HZ biogeochemical processes and agricultural irrigation return flow on nutrient dynamics and water quality at the watershed scale. In the future, mass transfer rate distributions will be prescribed as a function of hydromorphic features (Hou et al. poster), based on mechanistic hydrobiogeochemical simulations that are currently being conducted in various segments of the Hanford Reach (Bao et al. poster).

Poster #21-3

Spatio-Temporal Dynamics of km- to Reach-Scale Hydrological Exchange Flows along a Large Dam-Regulated River Corridor

Xingyuan Chen[1*], Xuehang Song[1], Pin Shuai[1], John Zachara[1], Glenn Hammond[2], Patrick Royer[1], Huiying Ren[1], Maoyi Huang[1], Jesus Gomez-Velez[3], Heping Liu[4], and Justine Missik[4]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]Sandia National Laboratories, Albuquerque, NM
[3]New Mexico Institute of Mining & Technology, Socorro, NM
[4]Washington State University, Pullman, WA

Contact: Xingyuan.Chen@pnnl.gov

BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of PNNL SFA seeks to study how the hydrological exchange flows (HEFs) at the river water and groundwater interface are impacted by the dynamics of river flow and the heterogeneity in hydrogeologic properties in dynamic river corridor systems. We used a combination of field observations and high-resolution 3D numerical simulations (PFLOTRAN) to understand the complex spatial and temporal dynamics of HEFs from the km- to reach-scale (10s of km) along the regulated river corridor of the Hanford reach. The spatially distributed hourly data acquired from a monitoring well network at the Hanford site are used to define the initial and boundary conditions of groundwater aquifer, as well as for calibrating and validating numerical models. The drilling logs of the wells and river bathymetry were used to conceptualize the hydrogeologic formations of the domain, which show substantial variability in aquitard topography within the Hanford river corridor. Spatially distributed river elevations simulated by the MASS1 model at an hourly time step were used as spatially-variable pressure boundary condition at the river. Heterogeneity in the riverbed conductance is parameterized based on the river substrate. Multiple numerical tracers are introduced at selected segments of river boundary to track the contribution of river water in the groundwater system from different locations of the river. Particle tracking is run by continuously releasing particles along the shoreline to reveal exchange pathways and estimate the distributions of river water residence time.

At the km-scale, the exchange pathways exhibit strong heterogeneity along the river shoreline within a given flow window as impacted the physical heterogeneity in riverbed substrate and in the aquifer. The riverbed permeability (or conductance) and its spatial heterogeneity are identified as the most sensitive parameters of the HEF model. The exchange patterns also vary substantially across different flow regimes. Consequently, the residence time distribution of river water in the groundwater system is characterized by long tails and multiple modes. The relationship between the residence time distribution and frequency of flow variation and physical heterogeneity is being developed. The km-scale model provided the foundation for building the reach-scale HEF model that encompasses multiple hydromorphic features of the entire reach, which is under active development. The HEF studies at both the km and reach scales and the subsequent studies on river corridor biogeochemical processes will fill in a critical need in bridging the gaps between hydromorphic-scale process understanding and robust predictions of the watershed hydrobiogeochemical function.

Poster #21-4

Hydromorphic Classification of the Hanford Reach through Integration of Field Observations and Hydrodynamic Models

Zhangshuan Hou[1], Huiying Ren[1], Chris Murray[1], Evan Arntzen[1], Xingyuan Chen[1], James Stegen[1], Maoyi Huang[1], Jesus Gomez-Velez[2], Zhuoran Duan[1], Bill Perkins[1], and Tim Scheibe[1*]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]New Mexico Institute of Mining and Technology, Socorro, NM

Contact: Tim.Scheibe@pnnl.gov

BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA is developing a new approach for classifying and mapping hydromorphic features in large, dynamic river systems. The approach will be used in modeling hydrologic exchange flows (HEFs) and biogeochemistry at local, reach and watershed scales. It is well known that HEFs are strongly controlled by the interaction of surface water flow dynamics with river morphology (hydromorphic features). We hypothesize that classes of hydromorphic features will exhibit distinct distributions of HEFs, subsurface residence times, and biogeochemical reaction rates. If this hypothesis is correct, large-scale classification and mapping of these features combined with field observations and numerical simulations of HEF characteristics will provide a pathway to develop reach- and watershed-scale models of hydrologic exchange and biogeochemistry based on widely available information such as LIDAR-based river bathymetry.

As a first step toward testing this hypothesis, we have developed and tested a new quantitative approach for classifying and mapping hydromorphic features based on field observations of river bathymetry and two-dimensional (2D) river flow simulations. This approach extends and combines a number of methods recently published in the geomorphology literature. We extracted several attributes of river bathymetry and flow on a highly-resolved 2D grid of the Hanford Reach of the Columbia River. Measures of riverbed bathymetry include Fourier spectra of elevation, local slope and aspect, and concavity/convexity. Flow simulations are from the 2D Modular Aquatic Simulation System (MASS2) model applied to a historical time period, which has been previously calibrated and validated for the Hanford Reach. Statistical methods including principal components analysis, K-means and expectation- maximization clustering, and information criteria were combined to identify four controlling variables that defined seven classes of hydromorphic features. When applied to the Hanford Reach, this classification scheme resulted in the identification of well-defined spatially coherent features that are physically interpretable and consistent over the entire reach, as well as sub-domains within the reach. Field ground-truthing and observations of riverbed textural properties are underway to verify and extend this classification scheme, and to compare the results to existing hydromorphic classification schemes. The resulting feature maps are being used to guide selection of sub-domains for mechanistic modeling of hydrologic exchange (Bao et al. poster) and novel biogeochemical reaction processes (Graham et al. and Song et al. posters); to guide the selection of locations for field studies (Stegen et al. poster); and to support development and parameterization of reach- and watershed-scale reduced-order models (Zhang et al. poster).

Poster #21-5

Three-Dimensional OpenFOAM-PFLOTRAN Coupled Model for Mechanistic Simulation of Hydrologic Exchange Flows in Varied Hydromorphic Settings

Jie Bao[1*], Yilin Fang[1], Xuehang Song[1], Xingyuan Chen[1], Maoyi Huang[1], Tian Zhou[1], Zhuoran Duan[1], Huiying Ren[1], Zhangshuan Hou[1], Glenn Hammond[2], and Tim Scheibe[1]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]Sandia National Laboratories, Albuquerque, NM

Contact: jie.bao@pnnl.gov

BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to develop three-dimensional models of coupled river hydrodynamics and subsurface fluid transport simulations in varied hydromorphic settings, for use in mechanistic reactive transport modeling and to support development of reduced-order models at system scales. Hydrologic exchange is a critical mechanism that shapes hydrobiogeochemical processes in river corridors and watersheds. Because of limitations in field accessibility, computational demand, and complexities of geomorphology and subsurface geology, three-dimensional mechanistic modeling studies to quantify hydrologic exchange flows (HEFs) have been mostly limited to local-scale applications in individual bedforms. Although it is well known that surface flow conditions, riverbed morphology, and subsurface physical properties strongly modulate hydrologic exchanges, quantitative measures of their effects on the strength and direction of such exchanges in complex hydromorphic settings are lacking. The open-source subsurface flow and reactive transport code PFLOTRAN has been used to model subsurface flow and reactive transport for hydrologic exchange studies, and commonly uses river water head as a boundary condition to drive the subsurface fluid transport, which assumes hydrostatic pressure on the river bed and neglects effects of dynamic pressure. Previous laboratory experiments and models have shown that pressure variations on the river bed induced by dynamic river flows can strongly impact hydrologic exchange. In this study, the open-source computational fluid dynamics (CFD) software OpenFOAM is used to model three-dimensional dynamic river flow and provide a more realistic pressure distribution on the river bed, through integration of the $k-\omega$ turbulence model and the volume of fluid (VOF) method. Assuming that HEFs do not affect surface water flow conditions because of their negligible magnitudes compared to the volume and velocity of river water, we developed a one-way coupled surface and subsurface water flow model that passes temporal and spatial varying pressure on the river bed derived from OpenFOAM CFD simulation to the subsurface model PFLOTRAN. The proposed three-dimensional OpenFOAM-PFLOTRAN coupled model is applied to the 7-km river section near Hanford 300A area, and used to quantitatively and systematically study the effects of river flow dynamic pressure induced on the HEFs and subsurface flow paths. Various hydromorphic settings that exist around the Hanford Reach are being classified and mapped (Hou et al. poster); the coupled model is being applied to a number of such settings to quantify the impacts of hydromorphology on HEFs and to develop information needed for reduced-order modeling at reach to watershed scales (Chen et al. poster).

Poster #21-6

Modeling Microbial Control of Historical Contingencies and Priming Effects in Biogeochemical Reactions

Hyun-Seob Song[1*], James Stegen[1], Emily Graham[1], Vanessa Garayburu-Caruso[1], and Tim Scheibe[1]

[1]Pacific Northwest National Laboratory, Richland, WA

Contact: HyunSeob.Song@pnnl.gov

BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to provide a mechanistic understanding of the microbial control exerted on biogeochemical dynamics for predictive biogeochemical process modeling. Biogeochemical reactions in the hyporheic zone often show nonlinear dynamics caused by the coupled effects of hydrology and microbiology. Key intriguing aspects of biogeochemical reactions identified by our SFA research include: 1) history-dependent response of microbial respiration to inundation (historical contingencies) and 2) priming effects observed only in a narrow range of mixing ratio between groundwater (GW) (containing relatively low concentration of thermodynamically favorable organic carbon) and surface water (SW) (containing relatively high concentration of recalcitrant organic carbon). Processes that govern these complex subsurface biogeochemical dynamics are yet poorly understood, and consequently poorly represented in current reaction network models. Towards revealing fundamental processes underlying historical contingencies and priming effects, we have developed two microbial community modeling approaches that view microbes and their interactions as key mediators of the complex biogeochemical functions mentioned above.

In the first model, we hypothesized historical contingencies as being driven by the dynamic interactions between two groups of microorganisms with distinct growth characteristics: copiotrophs (fast-growing organisms in high-carbon environments) and oligotrophs (slow-growing organisms adapted to low-carbon environments). The resulting model with copiotroph-oligotroph kinetics predicted the expected population trends and response time as a function of inundation frequency, indicating that historical contingencies in biochemical reactions can be controlled by the interspecies interaction in microbial communities as hypothesized.

In the second model formulated to simulate priming effects, we hypothesized that organic carbon in GW is protected by low concentration whereas organic carbon from SW sources is thermodynamically protected, but GW-SW mixing can simultaneously overcome both limitations. To test this hypothesis, we modeled a microbial community as a dynamic control system in which microorganisms optimally regulate enzyme synthesis to maximize the growth in a varying environment. This new model predicted mixing conditions for priming that matched our field observations, supporting our hypothesis by providing a plausible mechanism for overcoming both thermodynamic and kinetic limitations of carbon oxidation through GW-SW mixing.

To further test the model, we designed batch experiments to constrain interactions between concentration, chemical speciation, and thermodynamic properties in limiting hyporheic zone respiration (Graham et al. poster). This integrated modeling and experimental approach will generate new knowledge and understanding of key processes governing complex biochemical functions, which will then be translated into predictive reactive transport modeling for understanding system behavior across scales.

Poster #21-7

Interactions Between Organic Carbon Concentration, Chemistry, and Thermodynamics Govern Elevated Metabolism in the Columbia River Hyporheic Zone

Emily Graham[1*], Vanessa Garayburu-Caruso[1], Hyun-Seob Song[1], Malak M. Tfaily[2], Amy E. Goldman[1], Tim Scheibe[1], and James Stegen[1]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]Environmental Molecular Sciences Laboratory, Richland, WA

Contact: Emily.Graham@pnnl.gov

BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to understand the role of organic carbon chemistry in regulating aerobic respiration and to inform reactive transport models used in predictions of watershed-scale function. Organic carbon (C) metabolism is key to conceptualizing and parameterizing controls on biogeochemical cycling within reactive transport and watershed models. In particular, subsurface groundwater-surface water mixing (hyporheic) zones contain hotspots of enhanced metabolism that contribute substantially to river corridor function. Despite considerable research on biogeochemical reactions in the hyporheic zone, we still have a poor understanding of their governing processes. Previous work has shown a dependence of hyporheic biogeochemical rates on mixing of groundwater- (GW) and surface water- (SW) associated organic C pools with distinct chemistries. Based on these observations, we hypothesize that comparatively low metabolism in GW and SW independently are due to concentration limitation in GW (despite favorable C thermodynamics) and thermodynamic limitation in SW (despite sufficient C concentration). When GW and SW mix, we hypothesize both limitations are overcome, resulting elevated respiration.

To test these hypotheses, we evaluated the response of hyporheic zone sediments from the Hanford 300A in central Washington to different concentrations of carbon substrates with various chemical attributes. Four C compounds (two amino acids and two organic acids, one of each with high and low thermodynamic favorability) were added to batch reactors at ambient, 10- (equivalent to SW concentration), and 30-fold GW C concentrations. Further, mixed treatments including amino acids with varying thermodynamics were used to evaluate priming influences on respiration. Oxygen consumption was measured using non-invasive fiber opticsensors. Results indicate stimulated respiration when amino acids of differing thermodynamics are present in approximately equivalent proportions. Associated changes in geochemistry and in C chemistry provide mechanistic knowledge of possible thermodynamic limitations. Our results also support field-based insights suggesting a role for N-bearing compounds in metabolism.

Our results are being used to develop biogeochemical reaction models that incorporate multiple C compounds as electron donors (Song et al. poster). These models have replicated a priming-like effect within narrow mixing conditions observed *in situ*. Further, we lead a global initiative studying hyporheic zone metabolism through standardized sampling and a newly-developed sensor rod through the Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems project (WHONDRS, Stegen et al. poster). Collectively, this work links into reactive transport models that inform ecosystem predictions in the Columbia River watershed.

Poster #21-8

Local to Global Hydrobiogeochemical Impacts of High-Frequency Stage Fluctuations

James Stegen[1*], Tim Johnson[1], Amy Goldman[1], Xingyuan Chen[1], Emily Graham[1], Chris Strickland[1], Jon Thomle[1], and Tim Scheibe[1]

[1]Pacific Northwest National Laboratory, Richland, WA

Contact: James.Stegen@pnnl.gov

BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to understand the hydrobiogeochemical impacts of high frequency stage fluctuations from local-global scales through a research consortium and new sensors. While our understanding of dynamic river corridors is increasing, there is uncertainty in the hydrobiogeochemical impacts of high-frequency stage fluctuations, and such influences are omitted from current models. These deficiencies undermine predictions of feedbacks among energy-water systems, water quality, and river corridor health. The Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems (WHONDRS) aims to overcome these limitations. WHONDRS partners with researchers to use standardized methods across field sites to systematically collect and synthesize hydrobiogeochemical data in dynamic river corridors. By galvanizing a global community around understanding these impacts, WHONDRS will provide the scientific basis for improved management of dynamic river corridors throughout the world.

A key aspect of WHONDRS is the deployment of consistent instrumentation across field sites that is capable of estimating hydrologic exchange fluxes in very dynamic systems. Estimating these fluxes is essential for understanding and predicting hydrobiogeochemical processes, and requires understanding of pore velocity and mass flux. Current monitoring approaches estimate either transient pore fluid velocity or mass flux rate at the surface water/groundwater interface, but not both. To address this limitation, we developed a multi- sensor probe that continuously monitors the vertical distribution of pore fluid conductivity, temperature, pressure, and bulk electrical conductivity. Combined with fluid conductivity, bulk electrical conductivity estimates the vertical distribution of porosity, which links pore fluid velocity to mass flux. We developed the capability to simulate all time-series data from the probe using PFLOTRAN-E4D, and a joint Occam’s inversion for estimating the simplest vertical distribution of porosity, permeability, and dispersivity that honor the data. We have also developed a companion stochastic analysis to investigate uncertainty in parameter estimates and corresponding flux rates. Once parameters are estimated, transient pore fluid velocity and mass flux can be monitored using pressure boundaries at the top and bottom of the sensor probe.

The multi-parameter sensor rod is being developed, in part, to support WHONDRS efforts across globally distributed field sites. WHONDRS members will have access to this unique instrumentation and analytical software. WHONDRS, in collaboration with EMSL, is also supporting high resolution metabolomics to be paired with hydrologic exchange flux estimates. Collating hydrologic and metabolomic data across systems will reveal hydrobiogeochemical impacts of sustained high-frequency stage fluctuations from local to global scales.

Subsurface Biogeochemical Research

Oak Ridge National Laboratory
SBR Science Focus Area

Poster #21-23

Biogeochemical Transformations at Critical Interfaces Scientific Focus Area

Eric M. Pierce[1*], Baohua Gu[1], Scott C. Brooks[1], Scott Painter[1], Alex Johs[1], Dwayne Elias[2], Jeremy Smith[2], and Jerry Parks[2]

[1]Environmental Science Division, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: pierceem@ornl.gov

BER Program: SBR
Project: ORNL Critical Interfaces Scientific Focus Area (CI-SFA)
Project Website: http://www.esd.ornl.gov/programs/rsfa/

Over the last 3 years, the ORNL CI-SFA program has made substantial progress in fulfilling its Phase I (FY 2016–2018) objective of ***determining the fundamental mechanisms and environmental factors that control Hg biogeochemical transformations at critical interfaces in terrestrial and aquatic ecosystems***. Unique attributes of the CI-SFA include the range of spatiotemporal scales studied—spanning from molecular to watershed length scales and from picoseconds to seasonal variations in time—and the effective integration of technical expertise from widely varying science disciplines, including hydrology, geochemistry, microbiology, biomolecular sciences, high-performance computer simulations, and neutron science. This unique combination of scales and skills has resulted in a number of groundbreaking insights and discoveries, including the determination of importance of periphyton biofilms on net methylmercury (MeHg) production in East Fork Poplar Creek (EFPC) (Olsen et al., 2016; Olsen et al., in press). Although previous studies confirmed the prevalence of iron- and sulfate-reducing bacteria in EFPC sediments, our recent lab investigations demonstrated that changes to the carbon source impact microbial community composition and ultimately Hg methylation potential in EFPC sediment samples (Christensen et al., 2017). We have also determined computationally the permeability of Hg complexes through biomembranes (Zhou et al., 2017). We have discovered that certain methanotrophs and iron-reducing bacteria (e.g., *Geobacter bemidjiensis* Bem) are capable of degrading MeHg (Lu et al., 2017; Lu et al., 2016). Further, building on the discovery of the Hg methylation genes (*hgcAB*), we computationally probed the reaction mechanism for HgcA in MeHg formation (Johnston et al., 2016), designed *hgcAB* biomarkers (Christensen et al., 2016), and applied these probes to EFPC and to a range of other environmental systems in collaboration with US and international groups conducting Hg research. Leveraging our previous studies which established that dissolved organic matter (DOM) dominates aqueous Hg speciation in EFPC, we conducted the first-ever application of high-resolution mass spectrometry combined with quantum chemical calculations to confirm the molecular composition and structure of specific Hg-DOM complexes in EFPC (Chen et al., 2017) and evaluated the influence of EFPC derived DOM on Hg methylation by anaerobic bacteria (Zhao et al., 2017). Lastly, we have made substantial progress in developing our biogeochemical modeling framework for predicting Hg transformations in EFPC (Painter, submitted).

Poster #21-24

Kinetics of Mercury Methylation Revisited

Todd A. Olsen[1,2], Katherine A. Muller[1], Scott L. Painter[1], Grace Schwartz[1], and Scott C. Brooks[1*]

[1]Environmental Science Division, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Current affiliation: Geosyntec Consultants, Rancho Cordova, CA

Contact: brookssc@ornl.gov

BER Program: SBR
Project: ORNL Critical Interfaces Scientific Focus Area (CI-SFA)
Project Website: http://www.esd.ornl.gov/programs/rsfa/

Anthropogenic activities have disrupted the natural mercury (Hg) cycle releasing large amounts of this naturally occurring toxic element. The neurotoxin methylmercury (MeHg) is rarely a direct pollutant rather it is formed in the environment by a microbially mediated process known as mercury methylation. MeHg can also be demethylated via biotic and abiotic processes. To build models that predict MeHg levels in natural systems, scientists measure methylation and demethylation rates in laboratory experiments. We previously demonstrated that periphyton biofilms can be important sources of MeHg in East Fork Poplar Creek in Oak Ridge, TN (Olsen et al. 2016). Examination of our results and other published data sets suggested a new model of methylation/demethylation kinetics was needed because the data are typically analyzed using simple first-order rate expressions even though these data often exhibit kinetics that are inconsistent with first-order kinetic models. We hypothesized that apparent non-first-order dynamics in methylation/demethylation experiments was the result of competing kinetic reactions that reversibly converted Hg and MeHg to unavailable states. Using time-resolved measurements of filter passing Hg and MeHg during methylation/demethylation assays, a multisite kinetic sorption model, and re-analyses of previous assays, we show that competing kinetic sorption reactions can lead to time-varying availability and apparent non-first- order kinetics in Hg methylation and MeHg demethylation. The new model employing a multi- site kinetic sorption model for Hg and MeHg can describe the range of behaviors for time- resolved methylation/demethylation data reported in the literature including those that exhibit non first-order kinetics. Additionally, we show that neglecting competing sorption processes can confound analyses of methylation/demethylation assays, resulting in rate constant estimates that are systematically biased low. Simulations of MeHg production and transport in a hypothetical periphyton biofilm bed illustrate the implications of our new model and demonstrate that methylmercury production may be significantly different than projected by single-rate first-order models (Olsen et al., in press). Future work will seek to expand this model for application to metabolically active transient storage zones within the creek sediments.

References:
Olsen et al, 2016. Environ. Sci. Technol. 50, 10843-10850. Olsen et al, 2018. Environ. Sci. Technol. *In press*.

Poster #21-25

Effects of Natural Organic Matter and Minerals on Mercury Methylation

Linduo Zhao[1*], Xia Lu, [1] Shan Wu[1], Hongmei Chen[1], Eric M. Pierce[1], and Baohua Gu[1]

[1]Environmental Science Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: gub1@ornl.gov

BER Program: SBR
Project: ORNL Critical Interfaces Scientific Focus Area (CI-SFA)
Project Website: http://www.esd.ornl.gov/programs/rsfa/

Net methylmercury (MeHg) production in the environment is a result of complex interactions among Hg, microbes, natural dissolved organic matter (DOM), and minerals in water and sediments, but the mechanisms of these interactions remain poorly understood. We systematically investigated the effects of DOM and selected minerals on mercury [Hg(II)] methylation by an iron-reducing bacterium (FeRB) *Geobacter Sulfurreducens* PCA and a sulfate-reducing bacterium (SRB) *Desulfovibrio desulfuricans* ND132 under anaerobic conditions. The study was performed in laboratory incubations in a phosphate buffered saline (pH 7.4) either in the presence or absence of a DOM isolate from the contaminated East Fork Poplar Creek (EFPC) water and three distinct types of minerals (e.g., hematite, kaolinite, and smectite) with varying physico-chemical properties. We found that DOM effects on microbial methylation are bacterial strain-specific, time- and DOM-concentration dependent. Addition of small amounts of DOM (< 10 mg/L) inhibits Hg methylation by *G. Sulfurreducens* PCA but enhances Hg methylation by *D. desulfuricans* ND132 cells. The result implies that DOM likely enhances Hg methylation at such sites where SRB dominates but inhibits methylation in ecosystems where FeRB dominates. Interestingly, we also found that the presence of minerals, regardless of the mineral type, enhanced Hg(II) methylation by ND132 cells, and MeHg production increased by 2 to 4 fold. Results thus indicate that the sorption of both Hg(II) (freshly added) and cells on mineral surfaces may have favored cell uptake and thus methylation of Hg(II), although aging and drying of the minerals with the sorbed Hg(II) significantly decreased Hg(II) methylation. While exact mechanisms of the DOM- or mineral-enhanced Hg(II) methylation or DOM-inhibited methylation by *G. Sulfurreducens* PCA remain to be explored, these observations provide new insights into complex environmental geochemical factors influencing mercury cycling and methylmercury production in the aquatic environment.

Poster #21-26

Biogeochemical Mechanisms Affecting Mercury Species Transformation and Methylmercury Production or Degradation

Baohua Gu[1*], Xia Lu[1], Xiangping Yin[1], Wenyu Gu[2], Linduo Zhao[1], Alan A. DiSpirito[3], and Jeremy D. Semrau[2]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Dept. of Civil and Environmental Engineering, The University of Michigan, Ann Arbor, MI
[3]Dept. of Biochemistry, Biophysics and Molecular Biology, Iowa State University, Ames, IA

Contact: gub1@ornl.gov

BER Program: SBR
Project: ORNL Critical Interfaces Scientific Focus Area (CI-SFA)
Project Website: http://www.esd.ornl.gov/programs/rsfa/

The overall goal of this project is to gain a fundamental understanding of the key biogeochemical mechanisms controlling mercury (Hg) species transformation and methylmercury (MeHg) production or degradation in the aquatic environment. One of our most notable accomplishments last year was the discovery of a previously unrecognized MeHg demethylation pathway present in methanotrophs that differs from the organomercurial lyase pathway present in Hg-resistant bacteria. We found that some methanotrophs, such as *Methylosinus trichosporium* OB3b, take up and degrade MeHg rapidly, whereas others, such as *Methylococcus capsulatus* Bath, can take up but not degrade MeHg. Demethylation by *M. trichosporium* OB3b increased with increasing MeHg concentrations, but was abolished in mutants deficient in the synthesis of methanobactin, a metal-binding compound used by some methanotrophs such as *M. trichosporium* OB3b. Our results demonstrate hitherto an unknown, yet potentially widespread biological mechanism of MeHg uptake and demethylation due to the ubiquitous presence of methanotrophs in the environment, including the contaminated East Fork Poplar Creek (EFPC) in Oak Ridge, Tennessee. These findings may open new opportunities to explore how nature detoxifies MeHg in the environment.

Further, in addition to our studies of the effects of naturally dissolved organic matter (DOM) and minerals on Hg transformations (see abstract by Zhao et al.), we demonstrated a new pathway of abiotic photochemical formation of mercury sulfide (HgS or metacinnabar) from photolysis of the complexes of Hg and DOM, resulting in rapidly decreased Hg reactivity and availability for microbial uptake and methylation. Photo-irradiation of Hg-DOM complexes resulted in rapid HgS precipitation, loss of Hg reactivity, and decrease in MeHg production by the methylating bacterium *G. sulfurreducens* PCA. Loss of Hg reactivity proceeded at a faster rate with decreasing Hg/DOM ratio due to an increase in Hg binding with thiol functional groups on DOM. Our results suggest a potentially novel pathway of abiotic photochemical formation of HgS and explain a mechanism whereby freshly deposited Hg is readily methylated but, over time, progressively becomes less available for microbial uptake and methylation.

Poster #21-27

Molecular, Genomic and Physiological Studies of Mercury Methylation

Caitlin M. Gionfriddo[1*], Geoff A. Christensen[1], Ann M. Wymore[1], Mircea Podar[1], Anthony V. Palumbo[1], Craig C. Brandt[1], Ryan Harvey[2], Ally Soren[3], Cynthia C. Gilmour[3], Judy D. Wall[2], and Dwayne A. Elias[1]

[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Department of Biochemistry, University of Missouri, Columiba, MO
[3]Smithsonian Environmental Research Center. Edgewater, MD

Contact: eliasda@ornl.gov

BER Program: SBR
Project: ORNL Critical Interfaces Scientific Focus Area (CI-SFA)
Project Website: http://www.esd.ornl.gov/programs/rsfa/

The Microbiology team within the ORNL CI-SFA has made significant strides in understanding the Hg-methylation genes *hgcAB* from an ecological as well as from a biochemical standpoint. We have developed universal probes to better understand the diversity of organisms and environments harboring these genes along with clade-specific probes for quantification. The probes were tested against >30 pure cultures including 13 *Deltaproteobacteria*, nine *Firmicutes*, and nine methanogenic *Archaea* genomes. A distinct PCR product was confirmed for all *hgcAB* strains tested via Sanger sequencing. The clade-specific qPCR primers amplified *hgcA* and were highly specific for each clade. Recent improvements to the Firmicute qPCR protocol have allowed for a lower sensitivity, and we are currently testing reduced degeneracy (96 to 32-fold) in the universal probes to maintain diversity. To further validate these probes, we compared them to 16S rRNA sequences and both *hgcAB* and 16S rRNA sequences from metagenomes from eight mercury-contaminated sites. In both the metagenome and ORNL probe amplicon sequencing, *Deltaproteobacteria* dominated the Hg- methylator pool, and clade-specific qPCR probes were highly similar to the metagenomes, which showed that methylators and demethylators were abundant at low methylmercury (MeHg). Demethylators (estimated by *merB* abundance) but not sulfate-reducers (estimated by *dsrC* abundance) or methanogens (estimated by *mcrA* abundance) were abundant at high total Hg. These results suggest that high MeHg accumulation inhibits both methylators and demethylators. While *hgcAB* is predictive for methylating Hg, the abundance and widespread diversity suggests that *hgcAB* may provide a physiological function beyond Hg-methylation. Originally annotated as a carbon monoxide dehydrogenase (CODH) it has high sequence homology to the corrinoid iron-sulfur protein (CFeSp), and both act as methyl group carriers to generate acetyl-CoA. Since chloroform inhibited both CODH activity and Hg-methylation, we hypothesize that *hgcAB* codes for a membrane protein complex to form acetate from CO_2 for biosynthesis. We assayed organic acid metabolite and amino acid production from *D. desulfuricans* ND132 wild-type and associated mutants (Δ*hgc*AB, Δ*hgc*AB*::hgc*AB). All cultures were batch grown with pyruvate and fumarate. No differences in basic physiology (e.g., growth rate, cell yield, CO_2 or succinate production) were observed. Acetate production was ~2X higher in the wild type, supporting a role for the *hgc*AB gene product in the C1 metabolic cycle of *D. desulfuricans* ND132. The results of these studies will allow for more accurate identification and quantification of the Hg-methylators and will be essential in developing accurate and robust predictive models of Hg methylation potential.

Poster #21-28

Biomolecular Insights into Mercury Transformations

Jerry M. Parks[1*], Niranjan Govind[2], Andrew M. Graham[3], James C. Gumbart[4], Peng Lian[1,5], Anna Pavlova[4], and Jeremy C. Smith[1,5]

[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Environmental Molecular Sciences Laboratory, Richland, WA
[3]Grinnell College, Grinnell, IA
[4]Georgia Institute of Technology, Atlanta, GA
[5]University of Tennessee, Knoxville, TN

Contact: parksjm@ornl.gov

BER Program: SBR
Project: ORNL Critical Interfaces Scientific Focus Area (CI-SFA)
Project Website: http://www.esd.ornl.gov/programs/rsfa/

Decades of research have been devoted to understanding monomethylmercury (MeHg) formation and degradation, but little is known about the formation of dimethylmercury (DMeHg) in aquatic systems. We combined complementary experimental and computational approaches to examine the formation and decomposition of the binuclear bis(methylmercuric(II)) sulfide complex $(CH_3Hg)_2S$. We obtained a log K value of 26.0 +/- 0.2 for the reaction $2CH_3Hg^+ + HS^- = (CH_3Hg)_2S$. Thus, the binuclear $(CH_3Hg)_2S$ complex is likely to be the dominant MeHg species under high MeHg concentrations typically used in experimental investigations of MeHg degradation by sulfate-reducing bacteria. We provide evidence for slow decomposition of $(CH_3Hg)_2S$ to DMeHg and HgS, with a first-order rate constant $k = 1.5 \pm 0.4 \times 10^{-6}\ h^{-1}$. Quantum chemical calculations suggest that the reaction proceeds by a novel mechanism involving rearrangement of the $(CH_3Hg)_2S$ complex facilitated by strong Hg–Hg interactions that activate a methyl group for intramolecular transfer. Predictions of DMeHg formation rates under a variety of field and laboratory conditions indicate that this pathway for DMeHg formation will be significant in laboratory experiments utilizing high MeHg concentrations, favoring $(CH_3Hg)_2S$ formation. In natural systems with relatively high MeHg/$[H_2S]_T$ ratios, DMeHg production may be observed, warranting further investigation.

Microorganisms that produce MeHg use corrinoid cofactors to perform the methylation reaction. To enable accurate simulations of corrinoid-dependent systems, we developed CHARMM force field parameters for several corrinoids developed from quantum mechanical calculations. We provide parameters for corrinoids in three oxidation states, Co^{3+}, Co^{2+}, and Co^{1+}, and with various axial ligands. The resulting parameters were validated by assessing their agreement with quantum chemical calculations and by analyzing MD simulation trajectories of several corrinoid proteins for which X-ray crystal structures are available. In each case, we obtained excellent agreement with the reference data. This approach is readily adaptable for developing parameters for simulating other corrinoids or large biomolecules.

Poster #21-29

Unraveling the Cellular Biochemistry of Mercury Methylation

Swapneeta Date[1*], Katherine W. Rush[3], Stephen W. Ragsdale[3], Jerry M. Parks[2], and Alexander Johs[1]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[3]University of Michigan, Ann Arbor, MI

Contact: johsa@ornl.gov

BER Program: SBR
Project: ORNL Critical Interfaces Scientific Focus Area (CI-SFA)
Project Website: http://www.esd.ornl.gov/programs/rsfa/

Microbial mercury methylation is an enzyme-catalyzed process carried out by certain anaerobic bacteria and archaea. A two-gene cluster *hgcAB* is essential for mercury methylation and encodes a cobalamin-dependent membrane protein, HgcA, and a ferredoxin, HgcB, which are predicted to facilitate methyl transfer and cofactor reduction, respectively. The primary focus of our research is to determine the kinetics of the intracellular methylation reaction and rate-limiting steps. Additionally, we aim to identify metabolites and protein-protein interactions essential for the function of HgcA and HgcB. The metabolic pathways necessary for methylmercury (MeHg) formation by HgcA and HgcB are currently not well understood. To address this knowledge gap, we investigated one carbon metabolism, transport mechanisms and electron donors/acceptors in a series of methylating bacteria and archaea to gain insights into the cellular machinery associated with MeHg formation and to develop experimentally testable hypotheses. Furthermore, we developed a mercury methylation assay, which allows us to measure MeHg production in cell lysates of *Desulfovibrio desulfuricans* ND132 independent of cellular uptake processes. Our experimental results demonstrate that the competing abiotic Hg methylation reaction with methylcobalamin is negligible at neutral pH values (i.e., physiological conditions), which further illustrates that the catalytic effect of HgcAB is required in the biotic reaction. We have also determined the pH and temperature dependence of the biotic methylation reaction and calculated kinetic parameters and rates for the conversion of Hg(II) to MeHg using the Michaelis-Menten formalism. The concentrations of several intracellular components were varied to identify potential rate-limiting metabolites. Our collaborators at the University of Michigan expressed HgcB heterologously as a maltose binding protein fusion construct for characterization by spectroscopic methods and Hg(II) binding experiments. An ongoing Environmental Molecular Sciences Laboratory user proposal aims to identify conditions for HgcB structure determination by solution nuclear magnetic resonance spectroscopy. A detailed understanding of factors controlling the production of MeHg will improve the accuracy of predictive models and facilitate the development of strategies to reduce exposure to this pervasive neurotoxin.

Subsurface Biogeochemical Research

Lawrence Livermore National Laboratory
SBR Science Focus Area

Poster #21-19

The LLNL Subsurface Biogeochemistry of Actinides SFA

Annie B. Kersting[1], Mavrik Zavarin[1*], Brian Powell[2], James Begg[1], Yongqin Jiao[1], Harris Mason[1], Pihong Zhao[1], Zurong Dai[1], Claudia Joseph[3], Keith Morrison[1], Enrica Balboni[1], Nate Conroy[2], Corey Pilgrim[4], and Chad Durrant[1]

[1]Lawrence Livermore National Laboratory, Livermore, CA
[2]Clemson University, Clemson, SC
[3]Karlsruhe Institute of Technology, Germany
[4]University of California, Davis, CA

Contact: zavarin1@llnl.gov

BER Program: SBR
Project: SFA Subsurface Geochemistry of Actinides, LLNL
Project Website: https://doesbr.org/research/sfa/sfa_llnl.shtml

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 Thrust Areas: (1) **Fundamental Mechanistic Studies** that identify and quantify biogeochemical processes, (2) **Field Integration Studies** that investigate actinide transport characteristics, and (3) **Actinide Research Capabilities** that provide new opportunities for advancing actinide environmental chemistry. Here, we summarize the accomplishments from 2017 and 2018 and preview our research objectives for the coming years. We quantified the adsorption/desorption behavior of plutonium (Pu) on SWy-1 montmorillonite colloids. A model that incorporates known surface-mediated Pu redox reactions was developed and the resulting rate constants, in part, explain colloid-facilitated Pu transport on decadal timescales. Pu desorption experiments using colloids produced from hydrothermal alteration of nuclear melt glass revealed additional colloid associations that may exacerbate colloid facilitated transport and help explain observations at the Nevada National Security Site. Rates of $NpO_2(C_2O_3)_3^{4-}$ ligand exchange were measured using multinuclear NMR to determine exchange rates of an environmentally-relevant actinide organic ligand. Ligand exchange rates for the geochemically important $NpO_2(C_2O_3)_3^{4-}$ aqueous complex were measured and showed a distinct difference in the pressure dependencies for the uranyl and neptunyl complexes. We explored the redox reactions of PuO_2^{2+} and PuO_2^{+} with acetohydroxamic acid and desferrioxamine B. PuO_2^{2+} was instantaneously reduced to PuO_2^{+} but weak complexation with hydroxamate limited further reduction to Pu^{4+}. We performed cesium adsorption/desorption ternary (Cs+two minerals) experiments to study longterm sorption reversibility (500 days). The novel experimental approach using dialysis membranes revealed that slow desorption kinetics may play an important role in apparently irreversible Cs sorption. This approach will be applied to study slow desorption kinetics of actinides. The role of structural Fe on Pu(V) surface mediated reduction on montmorillonite was examined. The sorption rate was positively correlated with structural Fe. Comparison to other minerals indicates that surface mediated reduction rates can vary by as much as five orders of magnitude depending on the structure and composition of the surface. We examined U(VI) diffusion through bentonite over six years using a diffusion cell apparatus. Surprisingly, diffusion rates were about two orders of magnitude lower than values obtained in short-term experiments reported in the literature. The results suggest that long-term studies of key transport phenomena may reveal additional processes that can directly impact long-term actinide migration.

Poster #21-20

Desorption of Plutonium from Altered Nuclear Melt Glass Colloids

Enrica Baboni[1*], Claudia Joseph[2], Teresa Baumer[3], Kerri Treinen[1], Annie B. Kersting[1], and Mavrik Zavarin[1]

[1]Lawrence Livermore National Laboratory, Livermore, CA
[2]Karlsruhe Institute of Technology, Karlsruhe, Germany
[3]University of Notre Dame, Notre Dame, IN

Contact: balboni1@llnl.gov

BER Program: SBR
Project: SFA Subsurface Geochemistry of Actinides, LLNL
Project Website: https://doesbr.org/research/sfa/sfa_llnl.shtml

Radionuclides have been introduced into the environment and transported by groundwater at nuclear weapons testing sites, such as Nevada National Security Site (NNSS), USA. In the case of underground nuclear testing, the majority of the actinides that remain after the detonation are sequesterd in glass formed during the cooling of the plasma. Thus, the migration of residual plutonium (Pu) will be controlled by the rate of melt glass alteration. In particular, the nature of the Pu associated with secondary colloids produced as a result of glass alteration will have a significant impact on the transport behavior of Pu. To evaluate the nature of Pu association with glass alteration products, nuclear melt glass from NNSS was hydrothermally altered at 25, 80, 140 and 200 °C for about 1000 days. The degree of secondary colloid formation increased with increasing temperature, from no observable alteration—to almost complete. Smectite and zeolite colloids were identified by XRD in the 140 and 200°C samples. In follow-on experiments, long- term, flow-cell desorption experiments were conducted using the glass alteration colloids formed at 140°C and 200°C. The Pu desorption for the 140°C and 200°C experiments ranged from 7-15% and 1-8%, respectively. The Pu desorption behavior was simulated using a numerical model previously developed for Pu-montmorillonite adsorption/desorption (Begg et al., 2017). Pu desorption from the 140°C colloids can be predicted using our numerical model of Pu desorption from montmorillonite. However, Pu desorption from 200°C colloids is overestimated. This suggests that our numerical model of Pu desorption from montmorillonite may not accurately describe the behavior of colloids formed at higher temperatures. The results suggest that Pu desorption from melt glass colloids formed at 200°C is kinetically limited and/or irreversible. A fraction of the Pu in these materials may be permanently associated with colloids, possibly via structural incorporation, and may, as a result, have much greater migration potential. This apparent irreversibility helps to explain why trace levels of Pu are found in certain downgradient wells many decades after underground nuclear testing has ended.

Begg, J.D., Zavarin, M. and Kersting, A.B. (2017) Desorption of plutonium from montmorillonite: An experimental and modeling study. Geochimica et Cosmochimica Acta
197, 278–293.

Poster #21-21

Sorption Kinetics of Plutonium (V) to Three Montmorillonite Clays

James Begg[1], Mavrik Zavarin[1], Carina Edelman[2], and Annie Kersting[1*]

[1]Lawrence Livermore National Laboratory, Livermore, CA
[2]University of California, Santa Barbara, CA

Contact: kersting1@llnl.gov

BER Program: SBR
Project: SFA Subsurface Geochemistry of Actinides, LLNL
Project Website: https://doesbr.org/research/sfa/sfa_llnl.shtml

The sorption of Pu(V) to montmorillonite clay leads to the reduction of Pu(V) to Pu(IV) on the clay surface. In this project, the role of structural Fe on this reaction was investigated by quantifying Pu(V) sorption rates under atmospheric (oxic) conditions to three different montmorillonites with variable Fe content (SWy-1: 2.6 Wt % Fe; STx-1: 0.6 Wt % Fe; Barasym SSM: 0.01 Wt % Fe) at pH 4, pH 6, and pH 8. At all pH values, the sorption rate was positively correlated with structural Fe content. However, by 360 d, the extent of sorption was independent of Fe. Moreover, in the case of SSM (lowest Fe content) it was not apparent that sorption equilibrium had been achieved by the end of the experiment. The results indicate that at circumneutral pH, structural Fe will affect the kinetics of Pu(V) surface mediated reduction on montmorillonite but not necessarily the equilibrium Pu sorption affinity at environmentally relevant timescales. The differences in sorption rates and sorption extent on the three clays emphasize the need to perform long-term sorption experiments (> 1 year) to adequately capture the equilibrium processes controlling the uptake of Pu under oxic conditions. Comparison to other minerals indicates that surface mediated reduction rates of Pu(V) to Pu(IV) can vary by as much as five orders of magnitude depending on the structure and composition of the surface. The results highlight the confounding effect of Pu redox transformation kinetics on its observed behavior and the difficulties this causes for determining equilibrium values.

Poster #21-22

Long-term Aging of Actinide Solid Sources Exposed to Environmental Conditions

Melody Maloubier[1], Kathryn Peruski[1], Nathan Conroy[1], Hilary P. Emerson[2], Daniel I. Kaplan[3], Mavrik Zavarin[4], Annie B. Kersting[4], and Brian A. Powell[1*]

[1]Clemson University, Clemson, SC
[2]Florida International University, Miami, FL
[3]Savannah River National Laboratory, Aiken, SC
[4]Lawrence Livermore National Laboratory, Livermore, CA

Contact: bpowell@clemson.edu

BER Program: SBR
Project: SFA Subsurface Geochemistry of Actinides, LLNL
Project Website: https://doesbr.org/research/sfa/sfa_llnl.shtml

Exposure of actinide bearing solid phases to environmental conditions may result in a myriad of chemical or physical modifications including dissolution/precipitation, oxidation/reduction, and/or recrystallization/amorphization. Each of these reactions may have an impact on the long- term fate and transport of actinides in the environment. To better understand such processes, a series of field lysimeter experiments have been deployed to monitor the changes in chemical and physical properties of a variety of Pu and Np bearing solid phases including:

$Pu(V)NH_4CO_3(s)$, $Pu(IV)(C_2O_4)_2(s)$, $Pu(III)_2(C_2O_4)_3(s)$, $Pu(IV)O_2(s)$, $Np(IV)O_2(s)$, and $Np(V)O_2NO_3(s)$.

Lysimeters were deployed in triplicate to allow for destructive sampling after 2.5-4, 10 and 20 years.

To date, the 2.5-4 year sampling has occurred. X-ray absorption spectroscopy (XAS) of a $Pu(V)NH_4CO_3(s)$ source archived in an inert atmosphere and the same source recovered from field lysimeter indicates some reduction to Pu(IV) leading to the formation of $Pu(IV)O_{2+x}$ in both cases. However, solvent extraction of the archived source indicates that around 40% of the source remained in as Pu(V) while the field-deployed source contained less than 10% Pu(V). Thus, source reduction was accelerated when exposed to environmental conditions. Migration of Pu from a $Pu(IV)O_2(s)$ source was much lower than the migration observed in previous field lysimeter experiments using $Pu(VI)O_2(NO_3)_2(s)$. However, a small fraction of Pu is believed to have migrated due to transport of colloidal species.

Of the four lysimeters containing $Pu(V)NH_4CO_3(s)$ sources, two were placed in soil amended with 10% natural organic matter (NOM by weight). Relatively little transport of Pu has been observed with greater than 95% of the plutonium remaining within the source. However, the lysimeter containing 10% NOM exhibited less transport than the unamended lysimeter indicating that sorption to NOM or formation of ternary complexes could be retarding Pu transport.

Complementary laboratory studies have been performed to examine the role of NOM. Batch sorption experiments examining the influence of citric acid on Pu sorption to goethite and gibbsite suggest the formation of ternary mineral-NOM-Pu complexes that enhance Pu sorption at low pH. Similar ternary complexes are hypothesized to influence Pu migration in the field experiments. Reactive transport models based on the Pu-NOM-mineral experiments are under development.

Subsurface Biogeochemical Research

Argonne National Laboratory
SBR Science Focus Area

Poster #21-45

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

Kenneth Kemner[1*], Dionysios Antonopoulos[1], Theodore Flynn[1], Christopher Henry[1], Pamela Weisenhorn[1], Maxim Boyanov[2], Bhoopesh Mishra[3], Carlo Segre[3], Drew Latta[4], Michele Scherer[4], Daniel Kaplan[5], Dien Li[5], Nicole Martinez[6], Stephen Moysey[6], Brian Powell[6], Renata Rodriguez[7], Man Jae Kwon[8], Sen Yan[9], Paul Adams[10], Adam Arkin[10], Romy Chakraborty[10], Malak Tfaily[11], Edward O'Loughlin[1]

Underlined names are members of the new Argonne Wetlands Hydrobiogeochemistry SFA.

[1]Argonne National Laboratory, Argonne, IL
[2]Bulgarian Academy of Sciences, Sofia, Bulgaria
[3]Illinois Institute of Technology, Chicago, IL
[4]University of Iowa, Iowa City, IA
[5]Savannah River National Laboratory, Aiken, SC
[6]Clemson University, Clemson, SC
[7]Universidade Federal de Alfenas, Pocos de Caldas, Brazil
[8]Korea University, Seoul, Republic of Korea
[9]China University of Geosciences, Wuhan, P.R. China
[10]Lawrence Berkeley National Laboratory, Berkeley, CA
[11]Pacific Northwest National Laboratory, Richland, WA

Contact: kemner@anl.gov

BER Program: SBR
Project: Argonne National Laboratory SFA
Project Website: https://doesbr.org/documents/ANL_SFA_flyer.pdf; https://www.anl.gov/bio/project/subsurface-biogeochemical-research

Understanding the interplay of the Fe and S biogeochemical cycles with the hydrologic cycle is essential to accurately predict carbon cycling, nutrient availability, and contaminant mobility in near-surface and subsurface systems. The present objective of the Argonne SBR 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.* The Argonne SBR SFA has been integrating two key analytical strengths at Argonne—the Advanced Photon Source 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, Office of Biological and Environmental Research (BER) to "advance fundamental understanding of coupled biogeochemical processes in complex subsurface environments to enable system-level environmental prediction and decision support."

Recently, the Argonne SBR SFA has begun to incorporate a wetland field component within its ongoing research on Fe and S biogeochemistry in redox dynamic environments. Specifically, the Argonne SBR SFA is expanding into wetland hydrobiogeochemistry with a focus on a riparian wetland field site (Tims Branch) at the Savannah River Site. Research will center on major (e.g., Fe and C) biogeochemical cycles and their controls on water quality and contaminant (e.g. U) transport within the wetland, building on decades of expertise previously developed within the Argonne SBR SFA. The focus on hydrobiogeochemistry within a riparian wetland in the Southeastern US expands the portfolio of existing SBR SFA field sites concerned with watersheds, rivers, and streams in both arid and humid regions of the US that play a major role in controlling groundwater and surface water quality.

This newly focused Wetland Hydrobiogeochemistry SFA addresses two critical knowledge gaps: *(1) An in-depth understanding of the molecular scale biogeochemical processes affecting Fe, C, and contaminant speciation in wetland streams, sediments, and rhizosphere environments; and (2) An in-depth understanding of hyrologically-driven controls on the mass transfer of Fe, C, and contaminants within wetland streams, sediments, and rhizosphere environments.*

The long-term vision of the Argonne Wetland Hydrobiogeochemistry SFA is the development of a mechanistic understanding and ability to model the coupled hydrological, geochemical, and biological processes controlling water quality in many of the wetlands in the Southeastern US.

Poster #21-44

Effects of Fe(III) Inputs on the Rate of Methanogenesis in Wetland Sediment Microcosms

Theodore Flynn[1*], Lauren Johnson[1], Zena Jensvold[1], Maxim Boyanov[1,2], Kenneth Kemner[1], and Edward O'Loughlin[1]

[1]Argonne National Laboratory, Argonne, IL
[2]Bulgarian Academy of Sciences, Sofia, Bulgaria

Contact: tflynn@anl.gov, oloughlin@anl.gov

BER Program: SBR
Project: Argonne National Laboratory SFA
Project Website: https://doesbr.org/documents/ANL_SFA_flyer.pdf
https://www.anl.gov/bio/project/subsurface-biogeochemical-research

The presence of alternate terminal electron acceptors (TEAs) such as sulfate or ferric iron has previously been shown to inhibit methane production in transiently anoxic environments. This effect has been ascribed primarily to the ability of sulfate and iron reducers to outcompete methanogens for common electron donors (e.g., acetate, H_2) because, at standard state, respiration involving these TEAs provides a greater thermodynamic driving force compared to methanogenesis. In addition, evidence exists that methanogens can transfer electrons to ferric iron and dissimilatory metal reducers such as *Geobacter* have themselves been shown to transfer electrons directly to methanogens. The perceived role of competitive inhibition in controlling methanogenesis, however, is largely predicated on experiments where the production of methane was inhibited in microcosms that had ferric iron or sulfate present at the beginning of the experiment. In dynamic redox environments like wetlands, the formation of ferric iron is instead controlled by periodic influxes of O_2 into reduced sediments, so the impact of iron oxide addition on actively metabolizing methanogenic communities remains unclear.

We conducted microcosm experiments using sediment from a freshwater wetland amended with acetate. Shortly after the onset of methanogenesis, we amended each microcosm with ferric oxide: ferrihydrite, lepidocrocite, or goethite. We observed that the rate of methane production declined dramatically immediately following the addition of iron oxide despite the continued availability of acetate. The rate of acetate consumption also decreased significantly concomitant with the addition of ferric iron. Gas measurements also showed an immediate decrease in the partial pressure of H_2 in the headspace of microcosms following the addition of ferric iron. Greater inhibition of methanogenesis was observed with the less crystalline iron minerals ferrihydrite and lepidocrocite relative to the more crystalline goethite. X-ray diffraction showed the formation of the secondary ferrous minerals siderite and magnetite in ferrihydrite- and lepidocrocite-amended microcosms, but not in those amended with goethite. Unamended microcosms were dominated by 16S rRNA gene sequences classified as *Methanomicrobia*, a class of methanogenic archaea that comprised 32% of the total community during peak methane production. In iron-amended microcosms, however, these same taxa initially accounted for roughly 10% of the total community prior to the addition of ferric minerals, but sequences classified as *Geobacter* dominated soon thereafter. These results suggest that the impact of ferric oxides on methanogenesis is more complex than just thermodynamic limitations or kinetic inhibition and requires further study.

Poster #21-43

Redox Transformations of U, Hg, and As in Iron Oxide and Clay Systems

Maxim Boyanov[1,2*], Drew Latta[1,3], Michelle Scherer[3], Bhoopesh Mishra[1,4], Brittany Huhmann[3.5], Anke Neumann[3,6], Edward O'Loughlin[1] and Kenneth Kemner[1]

[1]Argonne National Laboratory, Argonne, IL
[2]Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, Bulgaria
[3]The University of Iowa, IA
[4]University of Leeds, Leeds, UK
[5]Massachusetts Institute of Technology, MA
[6]Newcastle University, Newcastle, UK

Contact: mboyanov@anl.gov; mboyanov@ice.bas.bg

BER Program: SBR
Project: Argonne National Laboratory SFA
Project Website: https://doesbr.org/documents/ANL_SFA_flyer.pdf
https://www.anl.gov/bio/project/subsurface-biogeochemical-research

Reactive Transport Models (RTMs) are often employed to predict the cycling of elements and the dispersal of contaminant plumes in natural environments. While RTMs can be based on *assumed* reaction pathways and empirical parameters, the transferability and the robustness of the model increase with the availability of mechanistic information that allows for the assignment of the *actual* reaction pathways, including the reactive species, products, and kinetics of the transformations operable in the system. Because model predictions are used to guide policy, improvement of RTMs translates directly into improved management and cost decisions.

The Argonne Subsurface SFA continues to provide the mechanistic understanding of processes needed for the improvement of RTMs. In the context of pollutant dispersal in groundwater, we studied the transformations of several dissolved contaminants (U, Hg, and As) in contact with reduced subsurface minerals (iron oxides and Fe-containing clays). In reactions of U^{VI} with reduced SWy-2 or NAu-1 clays we find that electron transfer occurs under the studied conditions (2-100 g/L clay loading, 250 μM U^{VI}, 2 mM bicarbonate, pH 7.2). However, the extent of U reduction and the reaction products depend on the type and amount of added clay. Using synchrotron x-ray spectroscopy (U L_{III}-edge XANES and EXAFS) we find that despite the stoichiometric excess of Fe^{II} in the system, U^{VI} is reduced to U^{IV} (uraninite) only at high solids loadings, whereas a mixed-valence U^V-U^{VI} oxide is stabilized at lower loadings. The results suggest that clay surfaces do not have sufficient high affinity sites for U^{IV} complexation that could prevent uraninite formation and that the formation of the mixed-valence U^V-U^{VI} oxide is controlled by the reducing capacity in the system. In reactions of Hg^{II} with reduced clays (4 g/L SWy-2 or NAu-1, pH 7.2 MOPS) the results of Hg L_{III}-edge XANES and EXAFS show that Hg^{II} is reduced to elemental Hg^0, independent of Hg concentration (0.1, 0.25, 0.5, and 1.0 mM), the presence of Cl- anions (0, 1, 10 mM), or the presence of a humic acid (0, 10, 20, 50, and 100 mg/L SWHA). Reduction to Hg^0 was also observed in the pH range 5.0-9.0. In reactions of As^V with the reduced iron oxide magnetite, the results of As K-edge EXAFS spectroscopy indicate that co-precipitation of dissolved As^V with magnetite leads to the formation of a stable, incorporated As^V species. The formation of such species may play a significant role in controlling As mobility in natural systems.

Poster #21-46

Elemental Content, U Redox Dynamics, and Microbial Communities in Wetland Sediment Cores from Tims Branch, Savannah River Site

Edward O'Loughlin[1*], Maxim Boyanov[1,2], Theodore Flynn[1], Daniel Kaplan[3], Dien Li[3], Brian Powell[4], Pamela Weisenhorn[1], and Kenneth Kemner[1]

[1]Argonne National Laboratory, Argonne, IL;
[2]Bulgarian Academy of Sciences, Sofia, Bulgaria;
[3]Savannah River National Laboratory, Aiken, SC;
[4]Clemson University, Clemson, SC

Contact: oloughlin@anl.gov

BER Program: SBR
Project: Argonne National Laboratory SFA
Project Website: https://doesbr.org/documents/ANL_SFA_flyer.pdf
https://www.anl.gov/bio/project/subsurface-biogeochemical-research

The Argonne SBR SFA is transitioning to the study of wetland hydrobiogeochemistry with a focus on a riparian wetland field site (Tims Branch) at the Savannah River Site in South Carolina. As a basis for understanding current conditions at the site, sediment cores (30 cm) and stream water were collected for analysis of elemental distributions, U speciation, and microbial community composition. To minimize changes to the native redox state within the sediment, cores were sealed and shipped to Argonne immediately after collection and were sectioned under anoxic conditions within hours of arrival the following day. The sediment profile consisted of a dark brown, organic layer (OL) on top of an organic matter depleted, mineral layer (ML). The OL was enriched in U (44.5±17.1 ppm) relative to the ML (6.38±2.19 ppm). U L_{III}-edge XAFS spectroscopy indicated that in the unsaturated portion of the OL, ~80% of the U was present as U^{VI}. In the saturated portion of the OL, however, >95% of the U was present as mononuclear U^{IV} that rapidly oxidized when exposed to air: 70% U^{VI}/Utotal was observed within three hours of exposure and > 95% after one month. U in the ML was predominantly U^{VI}. The cores contained diverse microbial communities, dominated by sequences from the phyla *Proteobacteria*, *Nitrospira*, *Chloroflexi*, and others. The stream water contained abundant reddish-brown flocs, consisting of Fe in the form of ferrihydrite (83%) and lepidocrocite (17%) as determined by Fe K-edge EXAFS spectroscopy. The flocs contained 320 ppm U, suggesting that they may provide a significant transport vector for U within the stream.

Stream water and core material were used to construct microcosms examining the effect of redox conditions (oxic versus anoxic) and C inputs (native C with and without a glucose amendment) on U speciation. Sediments incubated for 30 d under anoxic conditions showed >95% reduction to mononuclear U^{IV} regardless of the C input, whereas microcosms incubated under oxic conditions showed >95% U^{VI} regardless of C input. Anoxic microcosms generally showed an increase over time in fermentative (e.g., *Aeromonadaceae*, *Clostridiaceae*, and *Comamonadaceae*) and metal-cycling (e.g., *Geobacter* and *Geothrix*) organisms. Oxic microcosms were dominated by *Acidobacteriaceae*, *Sphingomonadaceae*, and particularly *Chitinophagaceae* sequences, which account for 20-40% of the total community in some microcosms.

Together these results demonstrate the potential for dramatic changes in U speciation/mobility with changes in the redox status of sediments at the Tims Branch site.

Subsurface Biogeochemical Research

SLAC
SBR Science Focus Area

Poster #21-51

SLAC Groundwater Quality SFA: Hydrologically Driven Biogeochemical Processes Controlling Water Quality

John Bargar[1*], Kristin Boye[1], Scott Fendorf[2], Christopher Francis[2], and Katharine Maher[2]

[1]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA
[2]Earth System Science, Stanford University, Stanford, CA

Contact: bargar@slac.stanford.edu

BER Program: SBR
Project: SLAC Groundwater Quality SFA
Project Website: https://www-ssrl.slac.stanford.edu/sfa/

A growing body of evidence highlights the importance of capillary fringe wet-dry cycling to groundwater quality in the upper Colorado River Basin (CRB), one of Earth's most over- allocated watersheds. Increasingly frequent drought is perturbing the timing and intensity of wet- dry cycles, creating a need for mechanistic understanding of water cycle-biogeochemistry linkages to support water quality prediction. Our research shows that wet-dry cycling in organic- enriched capillary fringe sediments creates transiently reduced zones (TRZs) at sites across the upper CRB. Ebbing summer water tables expose sediments that were formerly water-saturated to air, driving biogeochemical reactions that release organic carbon, nutrients and contaminants. Springtime re-saturation of sediments initiates a new suite of biogeochemical processes, which again have the potential to mobilize nutrients and contaminants. In this fashion, water and biogeochemical cycles intimately intertwine to control nutrient and contaminant behavior. At present, mechanistic understanding of the interdependencies between hydrology, biogeochemistry, and nutrient/contaminant transport within the capillary fringe is poor.

Here we present three sets of field observations that frame the new SLAC *Groundwater Quality* SFA and shed light on mechanisms of hydrologic-biogeochemical coupling in TRZs: (i) Downward as well as robust *upward* transport of water couples biogeochemical activity in the unsaturated zone, capillary fringe, and saturated zone throughout the year at the Riverton, WY site. Riverton is a model for saturated-unsaturated zone interactions, and these findings indicate that biogeochemical groundwater quality models must account for such vertical exchange processes; (ii) The intensity of reducing conditions in TRZs is thresholded by organic carbon and moisture content; and (iii) A reactive pool of iron in TRZs cycles between mackinawite and goethite during wet-dry redox cycles, providing an engine to periodically release or trap associated organic matter, nutrients, contaminants, and colloids. These findings suggest a new conceptual model wherein capillary fringes function as biogeochemical hot zones throughout the year, and nutrient and contaminant mobility is tightly coupled to iron cycling. The model predicts that solutes and nutrients accumulate in the soil zone during the summer and are flushed downward in spring, stimulating biogeochemical redox activity and mineral precipitation/dissolution in underlying saturated sediments. The mission of the SLAC Groundwater Quality SFA is to test this model through laboratory and field research, and to develop fine-scale quantitative process representations that can be incorporated into larger-scale models. We are initially focusing on modeling linkages between hydrology and redox conditions. Nutrient and contaminant mobilization will be understood within this framework.

Poster #21-52

SLAC Groundwater Quality SFA: Biogeochemical-Hydrologic Coupling in the Capillary Fringe at the Riverton, WY Site

Callum Bobb[1], Kristin Boye[2], Vincent Noël[2], Katharine Maher[1], Kenneth Williams[3], and John Bargar[2]

[1]Earth System Sciences, Stanford University, Stanford, CA
[2]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA
[2]Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: cabobb@stanford.edu

BER Program: SBR
Project: SLAC Groundwater Quality SFA
Project Website: https://www-ssrl.slac.stanford.edu/sfa/

Seasonal and synoptic hydrological changes in the Western U.S. drive complex and spatially- temporally variable biogeochemical transitions within the capillary fringe, with profound implications for groundwater quality. Springtime saturation of the capillary fringe triggers the onset of reducing conditions, which mobilizes iron and associated organic carbon and nutrients, initiates denitrification, and can drive reductive immobilization of sulfide-hosted and redox- active contaminants. Ebbing late-summer water tables expose formerly water-saturated sediments to air, oxidizing the accumulated reduced species and again impacting the mobility of contaminants. Thus, capillary fringe ecosystems mediate the coupling of water and biogeochemical cycles to govern the fate of contaminants of significance to water quality and management. However, our ability to scale hydrologic-biogeochemical coupling in capillary fringe transiently-reduced zones (TRZs) is limited, particularly between the fine (pore/micrometer) and meter scales. In particular, little is known about soil moisture thresholds that regulate successive biogeochemical reducing regimes, active N cycling pathways, contributions from microsites, and mechanisms of metal and radionuclide mobilization, yet these subjects are central to assessing the impact of biogeochemical transitions on water quality.

To address these needs, we characterized biogeochemical transitions in the capillary fringe at the former uranium ore processing site at Riverton, WY and are developing numerical representations of the key biogeochemical processes. Pairing porewater and sediment compositions with groundwater elevations over the course of a full snowmelt-driven runoff-to- drainage cycle, we observe coincident shifts in water level, redox potential, and contaminant concentrations. As spring runoff fully saturates the aquifer, a reducing front propagates upward through the soil profile, reaching a steady state within six weeks of the flood event. Reducing conditions are reflected in the porewater for nearly three months after reaching steady state. Rapid oxidation recovers the initial oxidized state within four weeks, suggesting that the rate of oxidation is more rapid than the onset of reducing conditions. The persistence of reducing conditions suggests that accumulation of reduced species (e.g. iron sulfide minerals) during the transient reduced phase serve as a redox buffer as the soil drains and is exposed to air, whereas the rapid re-oxidation suggests a threshold in soil moisture controls oxidation. These results are crucial to understanding redox-active capillary fringe behavior within the Western U.S. This research is further laying the groundwork for modeling contaminant mobility within these hydrologically active alluvial sediments.

Poster #21-53

SLAC Groundwater Quality SFA: Microbial Niche Partitioning at the Soil-Groundwater Interface in Transiently Reduced Floodplains

Emily Cardarelli[1*], Kristin Boye[2], John Bargar[2], and Christopher Francis[1]

[1]Earth System Sciences, Stanford University, Stanford, CA
[2]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA

Contact: ecardare@stanford.edu

BER Program: SBR
Project: SLAC Groundwater Quality SFA
Project Website: https://www-ssrl.slac.stanford.edu/sfa/

The Intermountain West hosts a large number of uranium-contaminated legacy DOE ore processing sites. Our research at several sites have shown that they experience 'hot moments' driven by rainfall, inundation, and meter-scale seasonal water table rise/fall that notably impact subsurface biogeochemistry, particularly for C, N, S, and Fe species and alter redox conditions. Transitions between oxidizing and reducing conditions are accompanied by intense microbial activity, biogeochemical transformations, and increased nutrient and contaminant fluxes. Rewetting events make limiting labile substances newly accessible to primed microbial communities. Despite their importance, little is known about the structure and function of the microbial community at the soil-groundwater interface or the extent to which these communities are impacted by rapid changes in water saturation. Microbial biomass and diversity at the soil- groundwater interface exceeds bulk soil levels by orders of magnitude, however accessibility of these sediments have previously precluded their study beyond 30 cm depth. Furthermore, past studies have primarily examined bacterial and archaeal communities with 16S rRNA primer sets that separately target each domain, thereby limiting holistic interpretations of the overall microbial communities. Thus, depth-resolved knowledge of microbial community diversity and distribution within the subsurface is extremely limited, but is needed to understand biogeochemical perturbations initiated by the water cycle.

To address these knowledge gaps, we collected 82 soil samples from Riverton, WY, and 80 collectively from Naturita, CO, Grand Junction, CO, and Shiprock, NM that were retrieved from multiple cores extending to 6 m depth and represent variable connectivity with the adjacent rivers. We pair depth-resolved molecular characterization of the microbial communities with detailed geochemical measurements and present evidence that suggests niche partitioning in the subsurface is influenced by hydrologic transition regimes. We show that unsaturated and saturated zone sediment communities can be used as 'endmembers' to understand microbial community variability in the hydrologically- and redox-variable capillary fringe. This study also demonstrates that use of the modified V4-V5 primer set for 16S rRNA amplicon sequencing allows the simultaneous detection of diverse archaea and bacteria as well as rare groups in the subsurface. Forthcoming metagenomes from select depths will further elucidate the 16S trends described, provide insight into newly described taxa, and improve our spatial and temporal understanding of how microbial metabolisms adapt in response to hydrologic transitions. This work provides the foundation for more targeted studies of microbial function in the Riverton site capillary fringe during wet-dry transitions.

Poster #21-54

SLAC Groundwater Quality SFA: Contaminant Response to Hydrologic Transitions in Transiently-Reduced Zones

Vincent Noël[1*], Kristin Boye[1], Ravi Kukkadapu[2], Kenneth Williams[3], and John Bargar[1]

[1]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA
[2]Environmental Molecular Sciences Laboratory, Richland, WA
[3]Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: noel@slac.stanford.edu

BER Program: SBR
Project: SLAC Groundwater Quality SFA
Project Website: https://www-ssrl.slac.stanford.edu/sfa/

Biogeochemical processes that govern metal and radionuclide mobility are highly sensitive to forcing by the water cycle. In the upper Colorado River Basin (CRB), water-saturated organic- enriched alluvial sediments locally exhibit reducing conditions and accumulate inorganic contaminants such as U, Zn, and Pb. Our research has shown that these so-called 'naturally reduced zones' (NRZs) commonly reside within the capillary fringe and are episodically or seasonally exposed to transient wetting and drying conditions. Because air enters pore spaces during capillary fringe 'dry-down', fluctuating hydrological conditions cause oxidation of NRZ sediments, creating conditions favorable to contaminant release. For example, oxidation of relatively insoluble U(IV) to soluble U(VI), as occurs in NRZs in the upper CRB, is generally thought to be an important mechanism of uranium mobilization. Knowledge of the interdependencies between hydrologic variability, sediment redox cycling, and contaminant import and export is requisite to model short- and long-term impacts on groundwater quality.

In this study, we tracked Fe, S, and U speciation to characterize the impact of hydrologic variability on redox processes and uranium speciation and mobility within fine-textured NRZ sediments in the capillary fringe at the Shiprock, NM DOE legacy site. As we have observed at other sites in the upper CRB, our results show that reducing conditions are needed to accumulate U in sediments. Surprisingly, however, our findings dispute the expectation that U predominantly accumulates as U(IV) in reduced sediments. Rather, we found that U accumulates as U(VI) at equal proportion to U(IV). The high abundance of crystalline U(VI) in reduced sediments suggests that redox cycling is needed to promote its accumulation, contradicting the common idea that U(VI) is lost during oxidation of sediments. We propose a new processes model for uranium mobilization in redox-cycled sediments where air-sensitive U(IV) is converted to crystalline U(VI) via a pathway that requires both hydrologic and redox variability under low permeability conditions.

In a related study, we have begun to investigate Zn speciation and stability in redox-active floodplains along the Slate River, Gunnison Co. CO, where it occurs as a contaminant at high sediment loadings (exceeding 1,000 mg/kg). Results to date suggest that Zn(II) is associated primarily with clay minerals within the transiently reduced zone and primarily with sulfides in the saturated zone. These findings suggest that Zn is stable during average seasonal wet-dry cycles. However, prolonged drying of the saturated zone, *e.g.*, during extended drought, could mobilize Zn due to sulfide oxidation.

Subsurface Biogeochemical Research

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

Poster #21-11

Interoperable Design of Extreme-scale Application Software (IDEAS): A Family of Synergistic Projects Focused on Improving Scientific Productivity

M. Heroux[1], L. C. McInnes[2], J. D. Moulton[3], D. E. Bernholdt[4], X. Li[5], and the IDEAS team

[1]Sandia National Laboratory, Albuquerque, NM
[2]Argonne National Laboratory, Argonne, IL
[3]Los Alamos National Laboratory, Los Alamos, NM
[4]Oak Ridge National Laboratory, Oak Ridge, TN
[5]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: moulton@lanl.gov

BER Program: SBR
Project: IDEAS
Project Website: https://ideas-productivity.org/ideas-classic/

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 initial phase of the IDEAS Scientific Software Productivity Project, recently dubbed IDEAS-Classic, (https://ideas-productivity.org/ideas-classic) was jointly funded by the Offices of Advanced Scientific Computing Research (ASCR) and Biological and Environmental Research (BER). IDEAS-Classic worked to enhance scientific productivity by improving the productivity of software developers and the sustainability of software artifacts — through an interdisciplinary and agile approach centered on adapting modern software engineering tools, practices, and processes to build a flexible scientific software ecosystem.

IDEAS-Classic has leveraged three BER use cases to motivate and test agile software methodologies, and to improve compatibility among complementary packages through creation of the Extreme-scale Scientific Software Development Kit (xSDK). IDEAS-Classic has also spearheaded outreach, featuring the new Better Scientific Software (BSSw) community portal (https://bssw.io) and the webinar series (https://ideas-productivity.org/events/hpc-best-practices-webinars/). Building on this success, IDEAS has grown into a family of synergistic projects to improve scientific productivity by qualitatively improving software productivity and sustainability. This poster highlights three current projects.

IDEAS-ECP: In support of the Exascale Computing Project (ECP), we continue development, customization, and curation of agile methodologies; work with individual ECP teams through Productivity and Sustainability Improvement Planning; and expand content for the BSSw site.

xSDK4ECP: To help support the seamless combined use of diverse, independently developed software packages in ECP, the xSDK continues to grow. The third release of the xSDK in December 2017 included a total of seven numerical libraries and two domain packages (the Alquimia geochemistry interface and the PFLOTRAN subsurface application).

IDEAS-Watersheds: The three BER use cases (climate impacts on the upper Colorado river system; hydrology and soil carbon dynamics of the Arctic; and hydrologic, land surface, and atmospheric process coupling over the contiguous U.S.) continue to evolve, providing motivation, testing, and evaluation of agile methodologies. Recent advances include improvements in multiscale frameworks and leveraging interoperable components to provide new scientific capabilities. In addition, we explore the critical role and benefits of a dedicated software engineer to oversee development processes, code reviews, testing and code releases. See three IDEAS-Watersheds posters led by D. Dwivedi, S. Painter, and L. Condon.

Poster #21-12

Leveraging Software Interoperability and Benchmarking to Accelerate Model Development of Terrestrial Ecosystems - IDEAS Use Case 1

Dipankar Dwivedi[1], Zexuan Xu[1], D. Svyatsky[2], S. Molins[1], Erica Woodburn[1], B. Kallemov[1], J. D. Moulton[2], and C. Steefel[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Los Alamos National Laboratory, Los Alamos, NM

Contact: cisteefel@lbl.gov

BER Program: SBR
Project: IDEAS
Project Website: https://ideas-productivity.org/ideas-classic/

To advance a robust predictive understanding of multi-scale terrestrial ecosystems requires representation and coupling of all relevant processes in models. There are various codes that are capable of quantifying hydrological and biogeochemical response across scales with slightly contrasting modeling approaches, but none of these can currently handle the full problem. In this presentation, as part of the overarching goal of **I**nteroperable **D**esign of **E**xtreme-scale **A**pplication **S**oftware (IDEAS), we demonstrate interoperability between codes to improve software and ultimately scientific productivity. In particular, we summarize two activities: (1) quantify the stream concentration-discharge at the Copper Creek (CC) sub- catchment and Lower Triangle Region (LTR) of the East River catchment to showcase a new level of spatial and time resolution as well as process fidelity in the modeling of multi-scale terrestrial ecosystems; (2) use model intercomparison to benchmark capabilities and build confidence in the model results.

The CC and LTR are located in the East River catchment, which is a study site of the Berkeley Lab's Watershed Function SFA, in southwestern Colorado. The CC is a high elevation sub-catchment which contributes flow to the East River approximately 25% annually, whereas the LTR encompasses complex geomorphic units such as floodplain, hill-slope, and meanders of the East River. ATS-AMANZI, which supports process-rich coupled simulations using Arcos multi-physics framework, is used to simulate integrated hydrological processes, winter snowpack, and follow-up snowmelt that influence stream chemistry at CC and LTR. The Alquimia interface, an interoperable interface designed to provide biogeochemical processes to flow/transport models, is used to represent geochemical processes including chemical weathering of rock and solute transport as well as mineral precipitation and dissolution in the models. Preliminary simulation results at CC and LTR show that hydrologic flow paths and groundwater residence times are key controls of stream concentration-discharge relationships.

Model intercomparison focuses on understanding differences in fluxes estimated by various reactive transport codes because of the distinctions in their abilities to handle structured vs. unstructured meshes. Here, we use ParFlow, ATS-AMANZI, and Chombo-Watershed to model complex and highly resolved topography encompassing two meanders of the lower East River catchment. ParFlow and ATS-AMANZI use structured and unstructured meshes, respectively, while Chombo-Watershed use embedded boundary adaptive mesh refinement (AMR) based package for creating meshes. Simulation results of integrated hydrology show confidence in model results by three codes. In addition, efforts are underway to benchmark biogeochemical processes for the same model domain.

Poster #21-13

Modeling Across Scales while Maintaining Links to Laboratory and Fine-scale Field Investigations: Cases Studies using the Advanced Terrestrial Simulator

Scott L. Painter[1*], Ethan T. Coon[1], and Ahmad Jan[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;

Contact: paintersl@ornl.gov

BER Program: SBR
Project: IDEAS
Project Website: https://ideas-productivity.org/ideas-classic/

Representing the emergent effects of fine-scale processes and heterogeneities on system-scale behavior, a critical challenge for system-scale environmental simulations in general, is particularly difficult for process-rich simulations that attempt to maintain clear links to field and laboratory investigations. Three examples illustrate how system insights can guide the design of efficient multiscale strategies for addressing that challenge and how highly configurable software facilitates implementation of those strategies. We previously showed that the thermal hydrology of polygonal tundra could be efficiently simulated at scale using a novel spatial structure based on insights gained from fine-scale simulations (Jan et al. 2018). We describe an extension of that approach that recovers the large-scale effects of subgrid microtopography through use of subgrid models informed by fine-scale simulations. Significantly, this multiscale computational strategy enables decadal, catchment-scale simulations without simplifying the three-phase physics of freezing soil, thus maintaining a clear link to laboratory and site-scale investigations of those processes. The software advances required to implement the polygonal tundra use case were also leveraged in a second use case focused on reactive transport in stream corridors. In that application, a subgrid model is used at each channel location in a stream network to represent transport and multicomponent biogeochemical reactions in the hyporheic zone. By writing the subgrid model in Lagrangian travel time form, computationally demanding three-dimensional reactive transport simulations are replaced with the one-dimensional reactive transport simulations, where each represents an ensemble of trajectories in the hyporheic zone. That multiscale approach allows multicomponent biogeochemical reactions such as redox processes to be modeled at their native small scales while embedded in reach-to-watershed scale simulations. Well-established geochemical modeling tools can be used to represent the reaction system using the Alquimia interface (https://github.com/LBL-EESA/alquimia-dev) for coupling. We apply the approach to a hypothetical reactive tracer test and demonstrate that formation of anaerobic zones within the hyporheic zone can affect the scaling of reactive tracer breakthrough from the laboratory to the field. In the final example, we demonstrate how related ideas and software tools can accelerate computationally demanding integrated surface/subsurface hydrology simulations at watershed scales. Specifically, we describe a multi-scale domain decomposition strategy that exploits the weak coupling that naturally exists between subwatersheds to improve numerical performance.

Publications: Jan, A., E.T. Coon, S.L. Painter, R. Garimella, and J.D. Moulton. Comput Geosci (2018) 22: 163. https://doi.org/10.1007/s10596-017-9679-3.

Poster #21-14

Advances in Hyper-Resolution Integrated Modeling of the Continental US and Connections to the National Water Model

Laura Condon[1*], David Moulton[2], David Gochis[3], Steve Smith[4], Carol Woodward[4], Adam Atchley[2], Basile Hector[5], Danielle Tijerina[6], Mary Michael Forrester[6], Aubrey Dugger[3], Wei Yu[3], Katelyn FitGerald[3], and Reed Maxwell[6]

[1]Syracues University, Syracuse NY;
[2]Los Alamos National Laboratory, Los Alamos, NM;
[3]National Center for Atmospheric Research (NCAR), Boulder, CO
[4]Lawrence Livermore National Laboratory, Livermore, CA
[5]Institut des Géosciences de l'Environnement, Grenoble France
[6]Colorado School of Mines, Golden, CO

Contact: maxwell@mines.edu

BER Program: SBR
Project: IDEAS
Project Website: https://ideas-productivity.org/ideas-classic/use-cases/

Understanding water flow at the continental scale helps untangle critical questions at the energy-water nexus. Our team has developed a fully integrated groundwater-surface water simulation of the Continental US (CONUS). Building from our existing work, this year we have been (1) continuing experiments with our simulations of current 6.2 million square kilometer domain, (2) expanding the simulation domain to extend to the coastlines and encompass the entire contributing area of the continental US, (3) directly comparing ParFlow-CONUS and WRF-Hydro configured as the National Water Model (NWM) and (4) coupling ParFlow and WRF Hydro to facilitate integration with the NWM.

A suite of 1-4 degree warming scenarios have been simulated with the existing CONUS domain. Results from these tests are used to evaluate the role of groundwater surface water interactions in watershed response to warming stress. Additional simulations with more recent climate forcing data are also used to evaluate hydrologic impacts of insect infestation and compare to GRACE satellite observations. In parallel, we have also been developing the next generation domain, which is roughly 25% larger than previous simulations and includes the entire surface water domain of the National Water Model (NWM). The grid for the new domain is aligned with the NWM, and topographic processing ensures that stream segments are consistent between models to facilitate direct comparison of approaches. Here we present progress on the development and initialization of the ParFlow model for the new domain.

The NWM represents the state-of-the-art in operational water prediction, and coupling to ParFlow allows for exploration of additional flow processes important for understanding and modeling the nation's water resources. Collaborating with the IDEAS team, we are exploring the benefits of appointing a software engineer dedicated to facilitating best practices as we are work to couple ParFlow into the WRF-Hydro modeling framework (the platform for the NWM). This physically based approach is a significant advancement beyond the currently implemented conceptual baseflow bucket model within the NWM. We illustrate proof of concept for the PF-WRF-Hydro model on several test beds as well as comparisons between the NWM and the existing CONUS domain.

Subsurface Biogeochemical Research

University Awards

Poster #21-9

From universal scaling for flow resistance in vegetated channels to predicting algal bloom and the evolution of benthic algae in riverine systems at the reach scale

Ilenia Battiato[1*]

[1]Stanford University, Stanford, CA

Contact: ibattiat@stanford.edu

BER Program: SBR
Project: University Award

The impact of submerged vegetation on nutrients and contaminants distribution in rivers and streams has been generally overlooked in recent multiscale modeling efforts. Yet, submerged aquatic vegetation (SAV), that consists of rooted macrophytes and attached algae, acts as the regulatory layer between many hydrological and ecological functions. SAV plays a pivotal role in fluvial systems by (1) mediating and regulating the transport between surface waters and the hyporheic zone and (2) promoting biodiversity through the creation of spatial heterogeneity in the flow field. One common challenge in modeling flow and transport in vegetated rivers and streams is the lack of predictive models linking vegetation type and morphology with effective transport properties of the vegetative layer itself and its dynamic linkages to its surroundings (i.e. groundwater and surface waters). Furthermore, the impact of environmental conditions such as water temperature, nutrient availability, light, local hydrodynamics and near-bed fluxes on SAV biomass dynamics (e.g., growth, uptake and removal) has been hard to disentangle. While the availability of LiDAR and unmanned aerial vehicle (UAV) data has opened new opportunities to spatially characterize vegetated environments over large scales, it also has demonstrated the startling limitations of existing models in establishing a mechanistic connection between vegetation morphology, its function and coupled response to variable river and environmental inputs. Here we use a combination of analytical and numerical methods to understand the impact of morphologically complex canopies on friction factor and the dynamic coupling between momentum, mass and SAV biomass evolution in the Khors rover bent in Montana. First, we discover a universal scaling law that relates friction factor with canopy permeability and a rescaled bulk Reynolds number; this provides a valuable tool to assess habitats sustainability associated with hydro-dynamical conditions [1]. Second, we develop a 3D code, CladoFOAM, in the OpenFOAM framework, to model Cladophora biomass distribution at the 1.5 km long Khors bent of the Clark Fork river in Montana, where extensive measurements of spatiotemporal evolution of Cladophora coverage at the reach scale, as well as seasonal variations of river discharge, nitrogen input, river temperature, light penetration, and daily/nightly variations of respiration rates, are available. The code, which solves a system of 18 coupled PDEs and ODEs, is able to accurately model the yearly vegetation coverage evolution at the reach scale [2].

[1] S. Rubol, B. Ling and I. Battiato, "Universal scaling-law for flow resistance over canopies with complex morphology", Scientific Reports, Accepted, (2018).

[2] Ling, B., S. Rubol, I. Battiato, 'Predicting algal bloom: the evolution of benthic algae in riverine systems', In preparation for Submission to PNAS, (2018).

Poster #21-66

Geologic Structure of the East River Watershed, Elk Mountains, Colorado: A Preliminary View from New Airborne Geophysical Survey Data

Burke Minsley[1] and Lyndsay Ball[1*]

[1]U.S. Geological Survey, Denver, CO;

Contact: lbball@usgs.gov

BER Program: SBR
Project: University Award
Project Website: https://minerals.usgs.gov/science/metal-transport-characterization- mineralized-mountain-watershed/index.html

Geologic controls on groundwater flow, particularly in structurally and topographically complex mountainous terrain, can be difficult to quantify without a detailed understanding of the regional subsurface geologic structure. This structure can influence the magnitude of groundwater flow through the mountain block, which in turn impacts groundwater composition and the flux of metals and nutrients to near-surface ecosystems. The East River Watershed in the Elk Mountains of Colorado is a research area for numerous projects within the Watershed Function Scientific Focus Area, a number of which are directly related to shallow groundwater flow or ecosystem processes that may be influenced by deep groundwater fluxes. In support of these efforts and on-going mineral resource studies at the U.S. Geological Survey, a regional scale airborne electromagnetic, magnetic, and radiometric survey was conducted of the greater East River watershed in 2017. These data give a view of the regional geologic structure that is unprecedented in both resolution and spatial coverage. This presentation will show preliminary data highlighting the geologic structure of the upper few hundred meters underlying the greater East River watershed. From universal scaling for flow resistance in vegetated channels to predicting algal bloom and the evolution of benthic algae in riverine systems at the reach scale

The impact of submerged vegetation on nutrients and contaminants distribution in rivers and streams has been generally overlooked in recent multiscale modeling efforts. Yet, submerged aquatic vegetation (SAV), that consists of rooted macrophytes and attached algae, acts as the regulatory layer between many hydrological and ecological functions. SAV plays a pivotal role in fluvial systems by (1) mediating and regulating the transport between surface waters and the hyporheic zone and (2) promoting biodiversity through the creation of spatial heterogeneity in the flow field. One common challenge in modeling flow and transport in vegetated rivers and streams is the lack of predictive models linking vegetation type and morphology with effective transport properties of the vegetative layer itself and its dynamic linkages to its surroundings (i.e. groundwater and surface waters). Furthermore, the impact of environmental conditions such as water temperature, nutrient availability, light, local hydrodynamics and near-bed fluxes on SAV biomass dynamics (e.g., growth, uptake and removal) has been hard to disentangle. While the availability of LiDAR and unmanned aerial vehicle (UAV) data has opened new opportunities to spatially characterize vegetated environments over large scales, it also has demonstrated the startling limitations of existing models in establishing a mechanistic connection between vegetation morphology, its function and coupled response to variable river and environmental inputs. Here we use a combination of analytical and numerical methods to understand the impact of morphologically complex canopies on friction factor and the dynamic coupling between momentum, mass and SAV biomass evolution in the Khors rover bent in Montana. First, we discover a universal scaling law that relates friction factor with canopy permeability and a rescaled bulk Reynolds number; this provides a valuable tool to assess habitats sustainability associated with hydro-dynamical conditions [1]. Second, we develop a 3D code, CladoFOAM, in the OpenFOAM framework, to model Cladophora biomass distribution at the 1.5 km long Khors bent of the Clark Fork river in Montana, where extensive measurements of spatiotemporal evolution of Cladophora coverage at the reach scale, as well as seasonal

variations of river discharge, nitrogen input, river temperature, light penetration, and daily/nightly variations of respiration rates, are available. The code, which solves a system of 18 coupled PDEs and ODEs, is able to accurately model the yearly vegetation coverage evolution at the reach scale [2].

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[2] Ling, B., S. Rubol, I. Battiato, ‘Predicting algal bloom: the evolution of benthic algae in riverine systems’, In preparation for Submission to PNAS, (2018).

Poster #21-62

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

Martin Briggs[1*], Fred Day-Lewis[1], Lee Slater[2], Chen Wang[2], and Ken Williams[3]

[1]USGS Hydrogeophysics Branch, Storrs, CT
[2]Rutgers University, Newark, NJ
[3]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: mbriggs@usgs.gov

BER Program: SBR
Project: University Award

The shallow interface sediments that line surface water bodies can host beneficial bacteria that naturally filter contaminants from groundwater as it passes 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 precipitated within pores and on grain surfaces. These deposits of metal oxides, which are also observed in abundance within mine-impacted watersheds, act as “contaminant sponges” that sorb toxic compounds. 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 released. We have been studying interface sediment-related metal oxides in the laboratory and within mountain watersheds in Colorado to: (1) better understand how dissolved metals, carbon, and contaminants pass from groundwater to surface water, and (2) capitalize on the ability of natural systems to adsorb and sequester contaminants.

In Year 1 of our research at the East River SFA we used fiber-optic distributed temperature sensing (FO-DTS) along with hand-held and Unoccupied Aerial System (UAS)-based thermal infrared surveys to locate focused groundwater discharges to the East River corridor, Oh-Be-Joyful Creek, and Coal Creek; the latter two streams being mine-impacted. We found little evidence of direct groundwater discharge to the river over approximately 4 km of the East River; instead the floodplain seems
dominated by lateral exchanges through various meander bends and beaver ponds. A subset of these exchange points showed strong metal oxide deposition. These points were sampled for water chemistry, geophysical properties, and vertical flux rates. In contrast, the smaller mine-impacted streams had numerous direct groundwater discharges to surface water of varied type such as focused fracture flow and diffuse flow through organic-rich sediments.

Geophysical measurements may be sensitive to the metal oxides formed on and within anoxic interface sediments. We have performed extensive laboratory analysis of basic thermal and geophysical materials properties of metal oxide-impacted natural and synthetic (controlled coating) sediments. Our preliminary results indicate that the presence of metal oxides does not reliably induce a magnetic susceptibility response, but does modify the electrical polarization of grain surfaces. Electrical and thermal properties are highly influenced by grain size and sediment type. We plan to utilize this lab- based understanding to refine field geophysical techniques for the efficient spatial mapping of anoxic groundwater discharge zones to streams across the East River SFA.

Poster #21-18

Respiration in Hyporheic Zones: Connecting Mechanics, Microbial Biogeochemistry, and Models

M. Bayani Cardenas[1*], Xiaofeng Liu[2], Matthew H. Kaufman[1], Anna Turetcaia[1], Xingyuan Chen[3], Maoyi Huang[3], Emily B. Graham[3], Joseph Brown[3], and James C. Stegen[3]

[1]Geological Sciences, The University of Texas at Austin, Austin, TX
[2]Civil and Environmental Engineering, Pennsylvania State University, College Park, PA
[3]Pacific Northwest National Laboratory, Richland, WA

Contact: cardenas@jsg.utexas.edu

BER Program: SBR
Project: University Award

Rivers are the primary carbon and nutrient conveyors of terrestrial ecosystems. River channels however are not simply inert pipelines. They are hotspots for sink and source reactions with magnitudes just as important as the conveyance. Reduced organic carbon, for example, can be extensively respired by bacteria residing in sediment. Although this respiration process is widely known, it has eluded broad quantification and mechanistic prediction. This incomplete knowledge of the fluxes across the land-water- atmosphere continuum is necessary for calculating terrestrial carbon budgets from plot to ecosystem to global scales.

This investigation seeks to develop plot-scale predictive understanding of carbon respiration in the shallow subsurface of riverbeds, the area referred to as the hyporheic zone. It addresses the overarching question of: “What are the physical and biogeochemical factors controlling hyporheic zone respiration of organic carbon and how are these factors inter-related?” The key factors to be tested are: (1) river hydrodynamics and bed morphology, (2) physical heterogeneity of the sediment hydraulic properties, (3) chemical heterogeneity and bioavailability of particulate organic carbon (POC) within the sediment, (4) riverine dissolved organic carbon (DOC) concentration and its bioavailability, and (5) the microbial community structure. The above factors are being analyzed through advanced computational simulations and laboratory experiments based on field observations from the PNNL SBR-SFA.

The general approach to testing hypotheses to the questions above involves novel flume experiments paired with multiphysics simulations which couple turbulent flow in river channels, hyporheic flow in sediments and reactive transport of carbon and nutrients within both domains. Our team has made a few major steps already and these will be reported in this poster. These include: (1) Flume experiments with detailed flow, chemical, and microbial characterization (2) Fully coupled model (one continuous domain) of turbulent open channel flow and porous media flow with reactive transport developed in OpenFOAM.

Based on (1), we found distinct microbial signatures between oxic and anoxic zones of the hyporheic zone in the sediment. The results also show that the microbial community that grew in the flume is similar to those found in natural aquatic settings. From (2), the novel model is able to replicate flow and transport observations from detailed experiments and from models using more primitive coupling schemes. Our incipient efforts in the past few months have shown the potential for upcoming discoveries regarding how carbon is respired in the hyporheic zones of aquatic sediment.

Poster #21-58

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

Frederick Colwell[1*], Andrew Thurber[1], and Laura Lapham[2]

[1]Oregon State University, Corvallis, OR
[2]University of Maryland, College Park, MD

Contact: rcolwell@coas.oregonstate.edu

BER Program: SBR
Project: University Award

Shallow subsurface microbial and geochemical processes in watersheds are dynamic and responsive to seasonal and long-term environmental change. At high elevation or latitude, such changes may occur during winter months when normal sampling is impossible, impractical, unsafe, or may actually alter the processes being studied. Yet accurate modeling of biogeochemical parameters in the subsurface requires sampling that captures events and persistent cold climate trends. Gaps in current models exist where data have not been collected during extended snow or ice covered periods. Our exploratory study will test the hypothesis that during snow cover in the East River (ER) watershed, episodic excursions of microbial community structure and biogeochemical processes and concentrations will fluctuate from values extrapolated from pre- and post- snow time periods. Elemental and microbial cycles will remain active in the aquifer long after the surface has been covered with snow. Melt events will stimulate biogeochemical processes. Our goal is to demonstrate that data collected through these periods will fill gaps and improve reactive transport models of biogeochemical processes in watersheds. We are coordinating with ongoing studies at the ER site especially those that using reactive transport modeling to frame the biogeochemical processes occurring in the watershed. We describe preliminary work conducted to place the specially designed samplers into the East River and the Shumway well in early November 2017 so that sampling over the winter months can begin.

Poster #21-31

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

Jason D. Demers[1*], Joel D. Blum[1], Scott C. Brooks[2], and Elizabeth R. Crowther[1]

[1]University of Michigan, Ann Arbor, MI
[2]Oak Ridge National Laboratory, Oak Ridge, TN

Contact: jdemers@umich.edu

BER Program: SBR
Project: University Award

Historical and ongoing releases of mercury (Hg) have resulted in a legacy of Hg contamination in streambed sediment, streambanks, and floodplain soils downstream of the Y-12 National Security Complex (Y12), along the flow path of East Fork Poplar Creek (EFPC) near Oak Ridge, Tennessee. Much of the Hg associated with streambed sediments, streambanks, and floodplain soils resides in relatively insoluble fractions, and has thus been considered to have little impact on dissolved total Hg (THg) concentrations. However, recent studies comparing hydrologic discharge and THg flux from Y12 and Lower EFPC suggest that additional dissolved Hg from the hyporheic pore water or groundwater discharge may variably contribute as much as a third of downstream dissolved Hg loads during baseflow conditions. Thus, 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 floodplains, and groundwater) with hydrologic flux measurements in four gauged reaches of EFPC. This will enable us to establish an isotope mass balance that assesses the relative importance of dissolved Hg contributed to the stream across these critical interfaces.

During the first half of this project we have: (1) completed more than a full year of ~ monthly baseflow surface water sampling to characterize the seasonal variability in concentration, flux, and isotopic composition of dissolved Hg in each of four gauged reaches of EFPC; (2) installed infrastructure (semi-permanent piezometers) for sampling hyporheic pore water and secured access to groundwater sampling wells in four reaches of Lower EFPC; (3) collected three seasonal sets of high-volume hyporheic pore water and riparian groundwater samples from these four newly instrumented reaches along the flow path; and (4) developed sequential extraction methods for the isotopic analysis of legacy mercury potentially re- mobilized from streambed sediment. Here, we present: dissolved Hg concentration and Hg isotopic composition of all surface water, hyporheic pore water, and riparian groundwater samples analyzed to date; make mass balance assessments regarding legacy inputs of dissolved Hg to the stream water of EFPC; and provide an assessment of our sequential extraction method for the isotopic analysis of legacy mercury sources.

Poster #21-67

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

Hannah Naughton[1], Carolyn Anderson[2], Christian Dewey[1.3], Peter Nico[3], Markus Kleber[4], Scott Fendorf[1*], and Marco Keiluweit[2]

[1]Stanford University, Stanford, CA
[2]University of Massachusetts-Amherst, Amherst, MA
[3]Lawrence Berkeley National Laboratory, Berkeley, CA
[4]Oregon State University, Corvallis, OR

Contact: fendorf@stanford.edu

BER Program: SBR
Project: University Award

Floodplains are poorly understood and dynamic components of the global carbon cycle that not are 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.

Important controls on carbon cycling within soils and sediments are imparted by mineral/metal associations and microbial metabolic constraints imposed by the respiratory pathway, both of which further serve 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.

Using a combination of field-scale measurement with micro-scale laboratory experiments, we find that oxygen diffusion limitations lead to heterogeneous redox profiles, shifting microbial metabolism to less efficient anaerobic SOC oxidation pathways. Across the floodplain transect in the East River watershed we are examining, organic carbon bound to Fe(III) (hydr)oxides constitute the most appreciable C (and N and P) phase, particularly in deeper sediments. Additional laboratory incubations demonstrated that, because organic N and P are preferentially bound to easily reducible Fe(III) (hydr)oxides, these nutrients were mobilized under reducing (water saturated) conditions during flooding. Further, within saturated soils of the floodplain, thermodynamic constraints on microbial metabolism result in preferential utilize of organic carbon compounds. 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 shows 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. Dissolved oxygen and nitrate alleviate the metabolic constraint and result in rapid utilization of metabolically protected reduced carbon compounds.

Collectively, our results illustrate the combined, and dynamic, impacts of mineral-associations and metabolic controls on carbon and metal fate. The highly variable hydrology of floodplains leads to concomitant changes in biogeochemical processes within soils that ultimate control organic carbon, nutrients, and metal cycles.

Poster #21-50

On Sub-grid Scale Variations of Transpiration

Inez Fung[1*]

[1]University of California, Berkeley, Berkeley CA (

Contact: ifung@berkeley.edu

BER Program: SBR
Project: University Award

In a climate model in which the land surface is resolved typically at 25 km or more, the focus has been on bulk properties of ecosystem function and structure as they affect the atmosphere. Such a gridbox typically comprises a large number of plant species with various traits, as well as subsurface properties such as porosity and depth to bedrock (DTB). With DOE support, we have developed a stochastic parameterization of hydraulic conductivity that takes into account preferential flow through weathered bedrock (Vrettas and Fung, 2015), and applied the Richards Equation with the new parameterization to investigate the impact of subsurface water storage capacity (especially in the weathered bedrock) and rooting structure on the timing and magnitude of transpiration (Vrettas and Fung, 2017). Here we present an application of the approach to a landscape, using a compilation of DTB at 30 arcsec resolution (Pelletier et al., 2016) and distribution of tree species and associated properties. Rooting depth is calculated using estimates of crown volume of each tree species and climate variables (Schenk and Jackson, 2002); species-specific transpiration dependence on climate is taken from Link et al. (2004). Strategies for upscaling the heterogeneous structure and function to gridbox level will be discussed.

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Poster #21-17

Transport and Transformation of Particulate Organic Matter in Permeable Riverbed Sediments

Matthew Ginder-Vogel[1*]

[1]University of Wisconsin-Madison, Madison, WI

Contact: mgindervogel@wisc.edu

BER Program: SBR
Project: University Award

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.

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. Additionally in batch experiments, we have determined that isolated humic acids (HA) can also provide electron donating equivalents to drive dissimilatory iron reduction (DIR), while at the same time serving as electron shuttles that accelerate DIR. Evidence of this phenomenon was provided by the overrepresentation of putative genes coding for enzymes that break down complex lignocellulosic material and (to a lesser extent) aromatic compounds in experiments containing HA. The potential for microorganisms to utilize a small but significant portion of HA is consistent with the emerging view of soil organic carbon as a continuum of variably decomposable organic compounds. The next phase of our research will investigate longer-term (2-4 week) decomposition dynamics of POM in permeable sediments under advective flow.

Poster #21-16

Quantifying Distributed Exchanges of Groundwater with the Columbia River – Preliminary Results

Michael Gooseff[1*], Abigail Conner[1], and Xingyuan Chen[2]

[1]University of Colorado-Boulder, Boulder, CO
[2]Pacific Northwest National Laboratory, Richland, WA

Contact: michael.gooseff@colorado.edu

BER Program: SBR
Project: University Award

Streams and rivers receive groundwater from their surrounding contributing watersheds to generally increase channel discharge down the river network. The inflow of groundwater is typically invisible to the naked eye, yet the contribution of groundwater, dissolved solutes, and energy has important biogeochemical and ecological impacts on surface waters. The goal of this project is to determine whether there is a clear relationship between the water management activities within and beyond the river corridor (lands that contribute to rivers; i.e., lateral watershed areas) to the fluxes and locations of groundwater inflows to the river channel. We are developing a new approach to identify the locations of, and estimate the fluxes of contributing groundwater (i.e., groundwater inflow to rivers) along the Columbia River. This new approach relies on detecting water quality anomalies along the river bed – especially dissolved oxygen, temperature, and electrical conductivity – indicating locations of groundwater inflows to the channel. Our data collection platform collects these data and GPS position at high frequency (<1 min). River discharge measurements are made upstream and downstream of these groundwater discharge locations. Combined, these field data would then be used to estimate how much water is entering the river from the ground, based on two mixing models. Repeated throughout the irrigation and non-irrigation seasons, these measurements will be used to determine whether there is a relationship between the locations and/or magnitude of fluxes of groundwater inflow to rivers to irrigation activities in the lateral contributing area to each segment of the river. Here we present our findings from our first field campaign to collect data along a segment of the Columbia River, WA in February 2018.

Poster #21-56

Controls of Hydrological Connectivity on Dissolved Organic Carbon Export in a Seasonally Snow-Covered Watershed

Wei Zhi[1], Li Li[2]*, Jason Kaye[5], Wenming Dong[3], Wendy Brown[4], Jason Kaye[5], Carl Steefel[3], and Kenneth H. Williams[3,4]

[1]Department of Energy and Mineral Engineering, The Pennsylvania State University;
[2]Department of Civil and Environmental Engineering, The Pennsylvania State University; * denotes PI
[3]Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory;
[4]Rocky Mountain Biological Laboratory;
[5]Department of Ecosystem Science and Management, The Pennsylvania State University.

Contact: lili@engr.psu.edu

BER Program: SBR
Project: University Award

Biogeochemical reactions at the watershed scale release dissolved organic carbon (DOC), a key solute affecting nutrient cycling and surface water quality. Flushing behaviors have been mostly observed for DOC across different watersheds under diverse conditions. However, underlying mechanisms for such flushing behaviors are poorly understood. Our overall goal is to: 1) develop a watershed-scale hydro-biogeochemical model to enable the simulation of DOC and other microbially-mediated processes; 2) use data-model integration to understand key controls of the DOC behavior at the Coal Creek, which is a seasonally snow-covered watershed (53 km^2) located in the west central Colorado.

In this work, a physically-based bio module, bioRT-Flux-PIHM, has been developed on the basis of RT-Flux-PIHM. This new bio module adds a Monod-type subroutine to solve for microbially-mediated processes and thus enables us to simulate DOC and DOC-relevant species (e.g. nutrients, and organic-metal complexes) at the watershed scale. This bio module has been verified against the widely used subsurface reactive transport code CrunchTope on soil carbon and nitrogen processes.

The application of bioRT-FLUX-PIHM in the Coal Creek watershed show that hydrologic connectivity largely determines stream DOC dynamics by shifting the dominant flow pathways and the major DOC sources connected to the stream. Under dry and low connectivity conditions, stream DOC is mainly from groundwater with low DOC concentration; under snow-melting season with high connectivity, stream DOC is predominantly composed of soil water with high DOC concentrations. Responsive SOC reaction rate to hydrologic conditions is a key mechanism to maintain a flushing DOC pattern. Groundwater is an indispensable component to reproduce stream DOC dynamics under baseflow conditions. In summary, stream DOC dynamic is controlled by groundwater influx when the watershed is under low hydrologic connectivity (transport-limited); however, it is largely controlled by soil water reaction when the watershed is under high hydrologic connectivity (supply-limited). These results have important implications for understanding and predicting watershed response to changing hydrological conditions and solute export from land to water.

Poster #21-68

Subsurface Carbon Inventories, Transformations and Fluxes Across Gradients in Elevation and Moisture Within an Alpine Watershed

Kate Maher[1*], Matthew J. Winnick[1], Hsiao-Tieh Hsu[1], Sami L. Chen[1], Yuchen Liu[2], Jennifer L. Druhan[2], Corey R. Lawrence[3], and Kenneth H. Williams[4]

[1]Department of Earth System Science, Stanford University, Stanford, California
[2]Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois
[3]U.S. Geological Survey, Denver, Colorado
[4]Lawrence Berkeley National Laboratory, Berkeley, California

Contact: kmaher@stanford.edu

BER Program: SBR
Project: University Award

The interface extending from the top of the soil layer to the bottom of the water table is characterized by dynamic couplings among vegetation, the movement of water and an array of subsurface biogeochemical processes. This complex interface also contains the largest reservoir of terrestrial carbon (C), one that is highly sensitive to shifts in climate, vegetation, and the resulting hydrologic regimes. Within the LBNL SFA East River, CO watershed study site, we are studying belowground respiration and carbon fluxes and their dependence on *(1)* the timescales and length scales of moisture variability and *(2)* molecular-level changes in organic matter compositions due to differing plant inputs and climatic drivers. We are further developing modeling approaches that capture the dynamic response to external forcings (*i.e.*, soil moisture dynamics and plant communities).

We have characterized two microcatchment study sites at different elevations and life zones (2950 and 3500 m; upper montane and upper subalpine, respectively) using depth- resolved soil moisture and temperature sensors, soil gas wells and lysimeters paired with repeat surveys of soil CO_2 fluxes, above ground biomass and belowground soil carbon distributions. Using a combination of Fourier transform infrared spectroscopy (FT-IR) and bulk carbon X-ray absorption spectroscopy (XAS), we find substantial variability in organic carbon functional group abundances between sites at different elevations. Soils at lower elevation are predominantly composed of polysaccharides, while soils at higher elevation have more complex distributions, including substantial portions of carbonyl, phenolic or aromatic carbon. Soil CO_2 respiration rates also show complex seasonal patterns across sites, with the majority of CO_2 production in the shallow (ca. <40 cm) soil. Peaks in CO_2 production follow precipitation events, with larger pulses of CO_2 production associated with larger rainfall events. However, the relationship between CO_2 production and soil moisture appears complex and highly variable due to the combined effects of both autotrophic and microbial respiration. Incubation experiments utilizing multiple rewetting events also show a complex dependence on soil moisture. A model framework that captures the transition between active and dormant biomass can explain the incubation experiments and will be examined as a tool for partitioning the net belowground fluxes. Collectively, carbon inputs and speciation and their coupling to soil moisture provide fundamental constraints on subsurface respiration dynamics and their potential response to environmental variability.

Poster #21-47

Towards a Better Understanding of Water Stores and Fluxes: Model Observation Synthesis in a Snowmelt Dominated Research Watershed

Reed Maxwell[1*], Dave Gochis[2], Anna Ryken[1], Rosemary Carroll[3], Lindsay Bearup[4], and Ken Williams[5]

[1]Colorado School of Mines, Hydrologic Sciences and Engineering, Golden, CO
[2]National Center for Atmospheric Research, Boulder, CO
[3]Desert Research Institute, Reno, NV
[4]Bureau of Reclamation, Lakewood, CO
[5]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: rmaxwell@mines.edu

BER Program: SBR
Project: University Award

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. Water balances are sensitive to the amount of water stored in the snowpack (SWE) and the amount of water leaving the system in the form of evapotranspiration—two pieces of the hydrologic cycle that are difficult to observe and model in heterogeneous mountainous regions due to spatially variant weather patterns. 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. We compare model simulations to field observations to elucidate process performance combined with a sensitivity analysis to better understand parameter uncertainty. Observations from a meteorological station in the East River Basin are used to force the integrated hydrologic model, ParFlow-CLM. This met station is co-located with an eddy covariance tower, which, along with snow surveys, is used to better constrain the water, carbon, and energy fluxes in the coupled land-atmosphere model to increase our understanding of high-altitude headwaters systems. Preliminary results suggest the model compares well to the eddy covariance tower and field observations, shown through both correct magnitude and timing of peak SWE along with similar magnitudes and diurnal patterns of heat and water fluxes. Initial sensitivity analysis results show that an increase in temperature leads to a decrease in peak SWE as well as an increase in latent heat revealing a sensitivity of the model to air temperature. Further sensitivity analysis will help us understand uncertainty of snow-related and forcing parameters. Through obtaining more accurate and higher resolution meteorological data and applying it to a coupled hydrologic model, this study can lead to better representation of mountainous environments in all ESMs.

Poster #21-69

Phosphorus Speciation in Atmospherically Deposited Particulate Matter and Potential Impact on Terrestrial Soil Nutrient Cycling and Ecosystem Productivity

Ugwumsinachi Godwin Nwosu[1], Morgan Barnes[1], Stephen C. Hart[1], Asmeret Asefaw Berhe[1], John N. Christensen[2], and Peggy A. O'Day[1*]

[1]University of California, Merced, Merced, CA
[2]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: poday@ucmerced.edu

BER Program: SBR
Project: University Award

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 N-oxides 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. To investigate P speciation, sources, seasonal changes, and potential bioavailability of atmospherically deposited P to soil in mountain ecosystems, particulate matter (PM) was collected by passive sampling at high elevation sites in the East River Watershed (CO) study area (in collaboration with the LBNL Watershed Function SFA), and at high and low elevation sites in the Southern Sierra Critical Zone Observatory (SSCZO, CA) during two seasonal periods (Sept.-Oct. 2016 and April-Sept. 2017). Sized-fractioned PM samples were analyzed by bulk and microfocused XANES at the P K-edge. Aqueous extractions of PM were studied by 31-P NMR. Analysis of lead isotopes provided information about PM sources. Results from linear combination fits of XANES spectra indicated a mixture of organic and inorganic P species, with organic-P dominating samples from high elevation sites at both CA and CO (~80-95% of total P). Fit results showed that organic P was a mixture of either bulk or adsorbed inositol hexakisphosphate (IHP, also known as phytic acid or phytate), commonly derived from plants, and DNA-P, mostly as an adsorbed species. Results from NMR confirmed the presence of DNA-P in the soluble fraction in addition to monoester-P, pyrophosphate, and inorganic orthophosphate. The lower elevation SSCZO site had a higher fraction of inorganic P (~30-45%), mostly as hydroxyapatite or Ca-associated P. For comparison, soil samples collected at the SSCZO sites had concentrations of total P up to three times lower than PM samples, primarily as inorganic P species (Al-phosphate and clay-associated phosphate). Lead isotope ratios indicated strong seasonal differences in long-range PM input from Asian sources to the CO sites, varying from 0 to almost 60% Asian lead between fall and spring, respectively. These results indicate that organic P dominates in high elevation PM samples, and that seasonally variable long-range transport is an important PM source to mountain ecosystems. Identification of DNA-P in PM samples suggests a more reactive and bioavailable form of P than IHP that has not been previously identified as a significant P component of PM.

Poster #21-37

Characterizing Radionuclide Subsurface Transport from Lab to Field Scales Using Multidimensional, Real-Time Imaging Techniques

Brian A. Powell[1*], Timothy A. DeVol[1], Stephen Moysey[1], Lawrence Murdoch[1], Kyle Barber[1], Juan Caicedo[2], Heather Clifford[1], Christophe Darnault[1], Musa Danjaji[3], Mine Dogan[1], Nimisha Edayilam[1], Bryan Erdmann[1], Brennan Ferguson[1], Daniel I. Kaplan[1,4], Shyla Kulpis[1], Biting Li[1], Abdullah Al Mamun[1], Melody Maloubier[1], Nicole Martinez[1], Fabio Matta[2], Fred Molz[1], Dawn Montgomery[1], Ashley Pales[1], Kathryn Peruski[1], Steve Serkiz[1,4], Lindsay Shuller-Nickles[1], and Nishanth Tharayil[1]

[1]Clemson University, Clemson, SC
[2]University of South Carolina, Columbia, SC
[3]South Carolina State University, Orangeberg, SC
[4]Savannah River National Laboratory, Aiken, SC

Contact: bpowell@clemson.edu

BER Program: SBR
Project: University Award
Project Website: https://www.clemson.edu/centers-institutes/neesrwm/EPSCoR/

This abstract provides highlights on real-time imaging studies of radionuclide transport performed as part of a DOE Experimental Program to Stimulate Competitive Research (EPSCoR) Implementation grant in South Carolina. Our approach seeks to characterize the time and length scales over which non- equilibrium states are maintained by rate-limiting (or rate-enhancing) reactions between radionuclides and co-reactants due to interactions between physical mass-transfer processes (i.e., flow, advection, diffusion) and (biogeo)chemical reactions. Multidimensional tools capable of real time monitoring radionuclide mobility were used to monitor lab to field scale experiments.

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

1. *Development of novel 1D and 3D photon based measurement techniques:* Ex-situ, real-time 1D gamma ray analysis, 3D x-ray CT and, Single Photon Computed Tomography (SPECT) techniques have been used to examine Tc-99m transport through porous media. Data have demonstrated accumulation of Tc within reducing zones of heterogeneous redox environments and a very slow release of Tc into the aqueous phase.
2. *Quantifying flow in porous media using x-ray CT:* Transfer of mass between fast flow in macropores and slow flow in the soil matrix is an important control on the fate and transport of solutes. We show that CT imaging can be used to investigate film flow along macropores, non- uniform imbibition from macropores into soils, and complex filling processes that will ultimately be critical for controlling the movement of radionuclides through the soil as well as the reagents controlling the chemical environment.
3. *Examination of uranyl phosphate dissolution facilitated by biogenic ligands:* The influence of nutrient availability, plant roots and plant root exudates on preferential water flow have been examined using 3D x-ray computed tomography (CT) and 2D light transmission experiments. Results indicate that root exudates influence the wetting of soil surfaces and has a significant impact on preferential water flow. Microfluidics and flow-through batch reactor experiments verified mass transfer limitations of citrate associate with the mineral surface as the primary control of uranyl phosphate dissolution.
4. *Observations of radionuclide transport in field lysimeters:* Field based lysimeter studies of Tc-99 and Np-237 these ions 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.

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

Poster #21-38

Visualizing Macropore Flow Mechanisms using 4D X-ray Computed Tomography

Abdullah Al Mamun[1*], Stephen Moysey[1], Mine Dogan[1], Lawrence Murdoch[1], Brian A. Powell[1], and Timothy A. DeVol[1]

[1]Clemson University, Clemson, South Carolina

Contact: bpowell@clemson.edu

BER Program: SBR
Project: University Award
Project Website: https://www.clemson.edu/centers-institutes/neesrwm/EPSCoR/

Project Abstract:
Transfer of mass between fast flow in macropores and slow flow in the soil matrix is an important control on the fate and transport of solutes. Time lapse X-ray Computed Tomography (CT) scans provide a non-invasive and non-destructive way to examine fate and transport phenomena in a heterogeneous material in 4D (i.e. transient three-dimensional imaging). Infiltration experiments were performed on a reference column of homogeneous soil and on a soil column with a substantial network of desiccation cracks running the length of the soil. The experiments were conducted by continuously dripping water containing a non-reactive NaI tracer at the top of the dry soil; the initial applied flow rate was 0.12 mL/min, but was increased to 0.33 mL/min after approximately 7 hours. Throughout the experiments the columns were located within a preclinical CT scanner (MILabs, Netherlands) and imaged with high resolution (i.e. 80 micron) at 7 minute intervals to visualize the flow pattern and evaluate mechanisms associated with flow in both the macropore and matrix domains. Quantitative, time-lapse images of water content were obtained from signal intensity changes between the dry and wet CT scans for each column.

The homogeneous column demonstrated an infiltration behavior consistent with standard concepts of unsaturated flow in soils. In contrast, however, complex flow behaviors were observed in the column containing the cracked soil. At low infiltration rates, the flow was dominated by film flow through the macropores (i.e., cracks) with comparatively little imbibition from macropore to matrix. At high infiltration rates, the macropores filled with water and a higher imbibition rate occurred within the soil matrix. A variety of features were also observed that demonstrate complex interactions between the macropores and matrix. For instance, water content increases were observed in the matrix prior to activation of macropore flow, which is consistent with the need to increase local matrix pressures above the threshold air entry pressure of the macropore. Also visible were the formation of flow networks where individual macropores were connected via short flow paths in the matrix. Overall, the results show that the wetting of the soil is a complex process reflecting different contributions from downward infiltration through the matrix and lateral wetting from vertical macropores. These complex filling processes will clearly impact the movement of radionuclides through the soil by advection, but they also have implications for the delivery of reagents that control the chemical environment of the soil, which in turn regulates the mobility of radionuclides.

Poster #21-59

Quantifying Dynamic Water Storage in Weathered Bedrock from the Pore to Landscape Scale

Daniella Rempe[1*], Logan Schmidt[1], Mong-han Huang[2], Kristen Fauria[3], Jennifer Druhan[4], Baptiste Dafflon[5], W. Jesse Hahm[6], and William E. Dietrich[6]

[1]University of Texas at Austin, Austin, TX;
[2]University of Maryland, College Park, MD;
[3]Woods Hole Oceanographic Institute, Woods Hole, MA;
[4]University of Illinois, Urbana Champaign, Champaign, IL;
[5]Lawrence Berkeley National Laboratory, Berkeley, CA
[6]University of California, Berkeley, Berkeley, CA;

Contact: rempe@jsg.utexas.edu

BER Program: SBR
Project: University Award

Many uplands regions are characterized by shallow soils underlain by weathered and fractured bedrock. The extent to which water is dynamically stored in the weathered bedrock region as “rock moisture” has not been systematically explored, yet its misrepresentation in hydrologic and Earth System models may have significant consequences for predicting transpiration fluxes as well as the chemical composition of groundwater and streamflow. Limited case studies have identified that deeply rooted trees can use water stored in weathered bedrock to subsidize soil moisture, particularly in times of water stress, however, further characterization of the moisture dynamics of the weathered bedrock region are needed to quantify ecosystem sensitivity to environmental change. Here, we seek to develop a predictive, geomorphic framework for quantifying landscape-scale rock moisture storage by directly evaluating differences in weathering profile evolution and dynamic water storage across four sites. Using a combination of near-surface geophysics and drilling, we map the weathered bedrock region and quantify the moisture dynamics within it at three sites associated with the Eel River Critical Zone Observatory, and the East River SFA. In the first six months of the study we have initiated the measurement of catchment-scale erosion rate via cosmogenic radionuclide analysis to evaluate how the pace of landscape evolution impacts weathering profile development. Seismic refraction datasets have now been collected across all four sites and reveal differences in the depth and extent of weathering. To directly quantify dynamic rock moisture storage, we are measuring core-scale petrophysical and hydraulic properties of weathered and unweathered bedrock and conducting successive downhole logging in boreholes, where core and boreholes are available. By the end of 2018, core and borehole logging data will be completed at all four sites. Results of successive logging from two of the sites reveals significant differences in the magnitude and spatial distribution of water storage dynamics that should correspondence to the hillslope scale seismic profiles. Additionally, field-scale nuclear magnetic resonance (NMR) logging indicates that dynamic water storage may occur in both the rock matrix and fractures. Laboratory analyses of core samples are underway to further investigate how water storage is distributed at the pore scale. By characterizing the pore- to hillslope-scale distribution of water storage in weathered bedrock at four sites and placing the dynamic storage in the context of landscape and weathering profile evolution, we seek to develop a predictive framework for modeling water storage in weathered bedrock and its impact on the hydrologic cycle.

Poster #21-36

Collaborative Research: Natural Organic Matter and Microbial Matter and Microbial Controls on Mobilization/Immobilization of I and Pu in Soil and Water Affected by Radionuclide Release in USA and Japan

Peter H. Santschi[1], Chen Xu[1], Peng Lin[1], Kathleen A. Schwehr[1], Daniel I. Kaplan[2], and Chris M. Yeager[3]

[1]Laboratory for Environmental and Oceanographic Research, Department of Marine Sciences, Texas A&M University, Galveston, Texas
[2]Savannah River National Laboratory, Aiken, SC
[3]Los Alamos National Laboratory, Los Alamos, NM

Contact: santschi@tamug.edu

BER Program: SBR
Project: University Award

In collaboration with Japanese Universities, we carried our research targeting natural organic matter (NOM) compounds and microbial processes that are responsible for speciation and fate of different radionuclides in soils from Japan and the USA. NOM is among the key environmental factors that influences the fate and transport of radionuclides in the environment. While this has been known for decades, there still remains great uncertainty in predicting NOM-radionuclide interactions because of lack of understanding of radionuclide interactions with the specific organic moieties within NOM. Furthermore, radionuclide-NOM studies using modeled organic compounds or elevated radionuclide concentrations provide compromised information related to true environmental conditions. Thus, sensitive techniques are required not only for the detection of radionuclides, and their different species, at ambient and/or far-field concentrations, but also for potential trace organic compounds that are chemically binding these radionuclides. GC-MS, ESI-FTICR-MS and AMS techniques developed in our lab permitted us to define how two radionuclides, iodine (I) and plutonium (Pu), form strong bonds with NOM by entirely different mechanisms: I tends to bind to aromatic functionalities, whereas Pu binds to nitrogen (N)-containing moieties, likely, hydroxamate siderophores.

Microbially mediated chelation and incorporation reactions can control a number of radionuclides, leading to retardation or mobilization, depending on whether the carrier compound is in solution or particle-bound as a function of pH or redox conditions of the ambient environment as well as the molecular weight of the carrier itself (Santschi et al., 2017a,b). In a study with RFETS soils, Pu was found enriched in NOM fractions that contained elevated leves of polycarboxylated aromatic and condensed aromatic formulas. These fractions also contained greater abundancy of CHON-type COO formulas, than fractions with lower Pu concentrations. N contents increased with the progression of purification and coincided with the trend of Pu concentration (DiDonato et al., 2017).

Based on humic acid (HA) samples from 10 soils collected from around the world, solid state ^{13}C nuclear magnetic resonance (NMR), and C, N, and S elemental analysis, binding of low concentrations of Pu (10^{-14} M) was correlated to the concentration of carboxylate functionalities and N groups in the particulate and colloidal phases. The much greater tendency of Pu binding to colloidal HAs than to particulate HA has implications on whether NOM acts as a Pu source or sink during natural or man-induced episodic flooding (Lin et al., 2017). In a parallel study, uptake of six particle-reactive and/or redox-sensitive radionuclides (^{210}Pb, ^{234}Th, ^{7}Be, ^{59}Fe, ^{237}Np and ^{233}Pa) by 14 HA extracts was also investigated revealing the capacity of these HAs to bind strongly to these radionuclides, either in particulate or colloidal state of the HA in a mimicked groundwater slurry (Lin et al., 2018).

While the speciation of radionuclides (e.g., I) can be controlled by abiotic factors such as biogenic Mn oxides at low pH (Grandbois et al., 2018b), biotic factors extracellular enzymes, microbial metabolites and microbial processes that alter the chemistry (e.g. pH, redox conditions) of the immediate environment (Yeager et al., 2017). Grandbois et al. (2018a) showed that the activity of soil enzymes, such as oxidases and peroxidases, and microbial biomass (particularly that of the Acintobacteria) were both strongly correlated with upake of I at environmentally relevant concentrations in forest soils from different regions and continents.

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Poster #21-32

Methylmercury Uptake and Degradation by Methanotrophs: A Hitherto Unknown, but Potentially Important Environmental Process

Jeremy D. Semrau[1*], Baohua Gu[2], Wenyu Gu[1], and Xia Liu[2]

[1]Department of Civil & Environmental Engineering, University of Michigan, Ann Arbor MI
[2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: jsemrau@umich.edu

BER Program: SBR
Project: University Award
Project Website: http://emmb.engin.umich.edu/

The overall goal of this project is to fully characterize a hitherto unknown mechanism of methylmercury degradation performed by aerobic methanotrophs. Previous work in our laboratories has shown that aerobic methanotrophs, through the production of a novel metal chelator called methanobactin, can bind inorganic mercury (Hg[II]), and by doing so, substantially reduce Hg[II] toxicity. We have also shown that methanobactin can bind a much more toxic form of mercury, the neurotoxin methylmercury (MeHg). Recently, the PIs have found that methanotrophs expressing methanobactin are also able to demethylate significant amounts of MeHg. Unlike the canonical organomercurial lyase in Hg-resistant bacteria,
methanotrophs take up and degrade MeHg at environmentally relevant pH and Hg concentrations (i.e., picomolar to nanomolar), suggesting that methanotrophs likely play a critical role in controlling net MeHg production and toxicity *in situ*. However, although methanobactin is necessary for methanotrophic-mediated MeHg degradation, it is not sufficient as purified methanobactin binds, but does not degrade MeHg. That is, methanobactin appears to serve as "delivery" mechanism to enable demethylation of MeHg by an as yet unknown process. Given that methanotrophs are ubiquitous, there exists a critical gap in our understanding of mercury cycling as methanotrophs likely play an important, yet poorly characterized role in controlling MeHg concentrations and by extension, MeHg bioaccumulation. To address this fundamental gap, we will characterize: (1) the products of methanotrophic-mediated MeHg demethylation using ^{13}C-labled MeHg; (2) the mechanism of methanotrophic-mediated MeHg degradation using a suite of selective inhibitors as well as construction of mutants where genes potentially involved in MeHg degradation are knocked out, and (3) the role of methanotrophs in MeHg degradation at the mercury contaminated East Fork Poplar Creek (EFPC) site in Oak Ridge, TN.

Publication:
Semrau JD, DiSpirito AA, Gu W, Yoon S. 2018. Metals and methanotrophy. Appl Environ Microbiol. E02289-17. doi:10.1128/AEM.02289-17

Poster #21-55

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

J.O. Sharp[1]*, L. Leonard[1], K. Mikkelson[1,] E.L. Brodie[2], Z. Hao[2], K.H. Williams[2,] C. Gable[3], E. Coon[3] and A. Atchley[3]

[1]Colorado School of Mines, Golden, CO
[2]Lawrence Berkeley National Laboratory, Berkeley, CA
[3]Los Alamos National Laboratory, Los Alamos, NM

Contact: jsharp@mines.edu

BER Program: SBR
Project: University Award

Montane ecosystems within North America are experiencing a prolonged period of ecological stress resulting from large-scale insect infestation that has affected tens of millions of acres of forest. Repercussions are a concern for the local economy, ecological stability, and biogeochemical processes that can influence water resources, ecosystem function, and human health. The goal of this exploratory project is to isolate relative biogeochemical contributions of needle decay from rhizospheric processes in a perturbed forest ecosystem. To query potential mechanistic drivers, fallen needles under lodgepole and spruce trees from the Rocky Mountains of Colorado were harvested from the forest floor and transported to a montane ecosystem in Crested Butte during the Fall of 2016. The collection enabled a focus on needle chemistry variables of beetle-impacted spruce, non-impacted spruce, and non-impacted lodgepole pine. Defined masses of the needles were deployed in quadruplicate at three distinct elevations to observe the effects of temperature, accelerated snowmelt, and needle chemistry on carbon and nitrogen export into the atmosphere and hydrosphere. Over this past year the needles and underlying soil decay horizons were monitored with a focus on gas flux and soil water chemistry. Initial findings suggest that needle chemistry and seasonality influence gas flux with an observed peak in CO_2 production and CH_4 consumption during high moisture summer events. Gas flux above all three needle types was typically more pronounced than the needle-free controls with lodgepole needle deployments displaying the most significant shift. In contrast, aqueous pore water constituents in proximal soil horizons have shown few shifts based on needle chemistry. However, increased concentrations of DOC, TN, and SUVA were observed after induced snowmelt at 10,400’ when contrasted with a proximal natural snowmelt plot. These observations support prior work studying enhanced carbon and nitrogen export into adjacent water bodies after snowmelt. Ongoing work focuses on characterizing the needle composition after decay, microbial ecology shifts associated with variables of elevation and needle chemistry and increased resolution of gaseous and pore water measurements during high moisture summer events. This research has implications for carbon and nutrient export that could aid in the prediction of and preparation for shifts of ecosystem function in montane watersheds with respect to water quality, gaseous export, and forest recovery.

Poster #21-33

AQUA-MER Aqueous Speciation Database: A Web Resource for Multi-Scale Modeling of Mercury Biogeochemistry

Jeremy C. Smith[1,2*], Scott C. Brooks[1], Peng Lian[1], Deepa Devarajan[1], Luanjing Guo[1], Scott L. Painter[2], and Jerry M. Parks[2]

[1]University of Tennessee Knoxville, TN
[2]Oak Ridge National Laboratory, Oak Ridge, TN

Contact: jsmith@utk.edu

BER Program: SBR
Project: University Award

Multi-scale geochemical modeling is important for predicting the fate of metals in terrestrial surface and subsurface systems. Typically, experimentally determined stability constants (i.e., log *K*) are used to calculate speciation profiles and to predict transport and transformations in the environment. However, modeling mercury (Hg) biogeochemistry suffers from a lack of reliable experimental data. For instance, experimentally measured log *K* values for $Hg(Cys)_2$ vary by 10-20 log units. Furthermore, the log *K* value for aqueous HgS was not measured directly but was derived by extrapolating the values for CdS and ZnS. Uncertainty in log *K* values propagates nonlinearly through speciation models of aqueous chemical systems. Latin hypercube sampling from a normal distribution of log *K* values leads to highly skewed distributions of aqueous Hg-containing species concentrations. Thus, if uncertainty is not considered, speciation model output of concentrations deviate away from the modes of the distributions, or values of the highest probability. Quantum chemical calculations can be used to supplement missing thermodynamic data. We have developed protocols to calculate accurate thermodynamic constants for environmentally relevant molecular species. We have developed an aqueous Hg speciation database, *AQUA-MER*, which collects high-quality experimental data adherent to IUPAC standards, accurate computational data, and provides a web interface to perform multi-scale Hg biogeochemical modeling. Currently, the database includes three modules: experimental log *K* data, calculated log *K* data, and Hg speciation modeling. The Hg speciation module currently uses PHREEQC to calculate aqueous speciation profiles using thermodynamic constants from experimental data, computational data, or both. Further refinement of the database will provide a one-stop website for multi-scale Hg biogeochemistry studies. Future studies will focus on combining the atomistic models with a macroscopic continuum-scale modeling framework to predict the transport and transformation of Hg in the environment.

Poster #21-65

Preliminary Results of 2017 Drilling, Geophysical Logging, Geologic Mapping, and Geochemical Sampling Activities in Redwell Basin, Elk Mountains, Colorado

Andrew Manning[1*], Lyndsay Ball[1], Richard Wanty[1], Burke Minsley[1], Jeffrey Mauk[1], and Philip Verplanck[1]

[1]U.S. Geological Survey, Denver, CO

Contact: amanning@usgs.gov

BER Program: SBR
Project: University Award
Project Website: https://minerals.usgs.gov/science/metal-transport-characterization- mineralized-mountain-watershed/index.html

A host of drilling, sampling, and geophysical/geological data collection activities were performed during summer 2017 in Redwell Basin, an alpine tributary of the East River in the Elk Mountains, Colorado. Redwell Basin contains bedrock with extensive sulfide mineralization that produces both natural and mining-related acid-rock drainage. The central objective of our project is to characterize and quantify controls on the flux of water and metals in the basin's bedrock groundwater flow system. Surface geophysical surveys were conducted using multiple methods including transient electromagnetic sounding, electrical resistivity tomography, total-field magnetics, and relative gravity. Resulting subsurface information aided in the siting of wells. Drilling activities included drilling a bedrock borehole high in the watershed to a total depth of 81 m with nearly complete core recovery, open-hole packer testing to determine permeability at different depths, and installing a multi-level monitoring well in the hole with four different screen depths. A full suite of borehole geophysical logs were also recorded using standard tools, plus acoustic televiewer, full wave form sonic, and heat-pulse flowmeter. Sixteen shallow piezometers were installed to depths <2 m in both colluvium and bedrock (using a hand-held core drill) in groundwater discharge zones. About 40 water samples were collected from piezometers, adits, springs, and streams, and analyzed for major ion and trace element chemistry and stable isotopes of water. A subset was also analyzed for Sr isotopes and age tracers (tritium, sulfur hexafluoride, and noble gas isotopes). Rock samples were collected from the drill core and submitted for permeability/porosity, petrophysical, petrographic, X-ray diffraction, and other chemical analyses. Finally, geological data collection included outcrop mapping of hydrothermal alteration and brittle structures, as well as comprehensive logging of stratigraphy, structures, and mineralogy in the drill core. Acquisition of analytical results and data interpretation are ongoing, and preliminary results will be presented at the meeting.

Poster #21-57

Snowmelt Dynamics Influence the Distribution of Microbial Communities and Carbon Pools in a Riverbed Ecosystem

Michael J. Wilkins[1], Audrey H. Sawyer[1], Kenneth H. Williams[2], Casey M. Saup[1], Amelia Nelson[1], and Savannah Bryant[1]

[1]Ohio State University, Columbus, OH
[2]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: wilkins.231@osu.edu

BER Program: SBR
Project: University Award

The hydrology of upland catchments in the western US is dominated by seasonal snowmelt that generates peak river discharge in spring and early summer, and low flow conditions for much of the remainder of the year. These snowmelt events are tightly linked to large-scale biogeochemical perturbations within such watersheds. Terrestrial organic carbon and other solutes are exported from hillslopes to the river channel, while increases in river discharge alter patterns of hyporheic mixing and solute processing in the riverbed. To investigate how mixing processes across the hyporheic zone affect carbon and metal processing, both discrete sampling and continuous monitoring efforts have been employed around a characteristic meander on the East River, CO.

Depth resolved temperature probes have been used to infer temporal patterns of flux across the sediment-water riverbed interface. Results have revealed strong river water down welling during periods of snowmelt-linked high discharge that contrast with groundwater up-welling signals during base flow. These hydrologic dynamics exert a strong effect on riverbed pore water geochemistry and microbiology.

While more carbon is exported from the catchment during high flow conditions, the chemistry (and therefore lability) of the DOC pool changes significantly across seasonal time scales. During snowmelt and associated high river discharge, river water carbon chemistry is more homogenous. Due to river water down welling, this signal is distributed into riverbed pore fluids up to 60 cm depth. Contrastingly, under low flow conditions when up-welling groundwater has a greater influence in the riverbed, more diverse and potentially labile carbon compounds are detected in both pore fluids and river water. These mixing patterns also have implications for the riverbed microbiome; under up-welling conditions, microbial communities are more depth stratified, while greater depth-resolved mixing of populations occurs when river water penetrates into the riverbed. These coupled geochemical and microbiological shifts likely affect the rate and extent of carbon and metal processing

These observational data are being complemented by ongoing modeling efforts to understand (1) seasonal transport and degradation of different carbon pools in the hyporheic zone of an upland river, and (2) the influence of spatial patterns in hyporheic mixing on pore water chemistry and microbial communities. The data-enabled models will be used to explore scenarios of carbon processing under a changing climate in mountain watersheds, and better understand how hydrology influences the biogeochemical heterogeneity of streambed environments.

Poster #21-15

Microbial Ammonium Cycling is Critical to Nitrogen Transformations in Columbia River Sediments

LM Solden[1], EX Graham[2], W Nelson[2], D Hoyt[3], M Tfily[3], J Villa[4], G Bohrer[4], J Stegen[2], and KC Wrighton[1,4]

[1]Department of Microbiology, The Ohio State University, Columbus OH
[2]Pacific Northwest National Laboratory, Richland, WA, USA
[3]Environmental Molecular Sciences Laboratory, Richland WA, USA
[4]Environmental Science Graduate Program, The Ohio State University, Columbus, OH

Contact: wrighton.1@osu.edu

BER Program: SBR
Project: University Award

The hyporheic zone plays a major role in carbon and nitrogen fluxes in river systems, yet the microorganisms and their metabolic interactions mediating these processes are largely unknown. To address this knowledge gap, we performed metagenomic and metaproteomic analyses on sediment cores spanning depth and vegetative gradients adjacent to the Columbia River. To date we have reconstructed 20 near-complete genomes from the 6 most abundant and active lineages including members of *Nitrospira* (3 genomes), Thaumarchaeota (6 genomes), Actinobacteria (5 genomes), Aciduliprofundum, as well as novel members within the Deltaproteobacteria, Rokubacteria, and Armatimonadetes (3 genomes). Metabolic predictions from these genomes indicated that ammonium is central metabolite interconnecting nearly all the genomes. For instance, Deltaproteobacteria and Armatimonadetes genomes all encode the capacity to degrade amino acids providing a source of ammonium to system. This metabolite can then be oxidized by Thaumarchaeota to nitrite, which is subsequently oxidized to nitrate by *Nitrospira*, and regenerated to ammonium via dissimilatory nitrate reduction by Actinobacteria. Proteins involved in these predicted activities were detected in the metaproteomic data, confirming that active organic nitrogen fermentation, nitrification, and denitrification co-occur in the subsurface environment. Together our data indicate that nitrogen compounds are transformed by a network of specialists, cycling nitrogen in a modular fashion in the hyporheic zone.

Poster #21-34

Organic Carbon Stability During Fe Redox Reactions: Coupling Geochemistry, Microbiology and Field Monitoring

Yu Yang[1], Eric E. Roden[2], Daniel Obrist[3,4], Annie B. Kersting[5], and Baohua Gu[6]

[1]University of Nevada, Reno, Reno, NV
[2]University of Wisconsin, Madison, Madison, WI
[3]Desert Research Institute, Las Vegas, NV
[4]University of Massachusetts, Lowell, Lowell, MA
[5]Lawrence Livermore National Laboratory, Livermore, CA
[6]Oak Ridge National Laboratory, Oak Ridge, TN

Contact: yuy@unr.edu

BER Program: SBR
Project: University Award

In the past two years, we have coupled geochemistry, microbiology and field monitoring to study the stability and reactions of soil organic carbon during the redox reactions of iron (Fe) minerals.

Our geochemical analysis showed that organic carbon associated with pure phase iron (Fe) oxide minerals (hematite, ferrihydrite) and natural Fe oxides in soils was released to the solution phase in conjunction with the reduction of Fe(III). When natural soils were exposed to an anaerobic- aerobic transition, organic carbon respiration was negatively linked to the amount of poorly crystalline Fe-oxide-bound organic carbon, but positively with the crystalline Fe-oxide-bound organic carbon. These results suggest that generation of poorly crystalline Fe oxides during the re- oxidation processes potentially can sequestrate organic carbon. Other experiments showed that under aerobic conditions, binding with ferrihydrite inhibits the bioavailability of labile substrates such as glucose and formic acid.

We also showed the extracted organic carbon can serve as both electron donor and shuttle for the reduction of hematite and ferrihydrite. In the presence of extracted organic carbon, metagenomes from hematite-reducing cultures had an overrepresentation of genes involved in the degradation of polysaccharides and to a lesser extent aromatic compounds, suggesting complex OC metabolism. Genomic searches for the Porin-Cytochrome Complex resulted in matches to Ignavibacterium/Melioribacter, DIRB capable of polymeric OC metabolism. These results indicate that such taxa may have played a role in both Fe reduction and decomposition of complex OC in anoxic soils and sediments. Metagenomes from ferrihydrite-reducing cultures also showed enrichment of genes that may have contributed to the degradation of complex OC (i.e., lignocellulose) into simpler organic compounds that can serve as electron donors for Fe reduction.

For the tundra soil organic carbon dynamic monitoring, in situ observations of CH_4 and CO_2 concentrations were undertaken within and above the soils at the Toolik Field Station over a 2- year period. Field observations showed both net oxidation of CH_4 and production of CO_2 in tundra soils, and suggest that fluxes of both species from the soil are subject to different temperature sensitivities and hysteresis effects upon freezing and thawing. The dynamics of greenhouse gas emissions can potentially be linked to the redox fluctuations.

Collectively our project has provided unique integrative understanding about the biogeochemistry of organic carbon during the redox reactions of Fe.

DOE Scientific User Facilities and Related Resources

Poster #BF-Hall

Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) - A New U.S. DOE Data Archive

Deb Agarwal[1*], Charuleka Varadharajan[1], Shreyas Cholia[1,2], Cory Snavely[2], Valerie Hendrix[1], Fianna O'Brien[1], Abdelrahman Elbashandy[1], Dan Gunter[1], William Riley[1], Chris Jones[3], Matt Jones[3], Amber E Budden[4], and Dave Vieglais[5]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]NERSC, Berkeley, CA
[3]NCEAS, Santa Barbara, CA
[4]DataONE, Santa Barbara, CA
[5]University of Kansas, Lawrence, KS

Contact: daagarwal@lbl.gov

BER Program: CESD Data Management
Project: ESS-DIVE
Project Website: http://ess-dive.lbl.gov

The ESS-DIVE archive is a new U.S. Department of Energy (DOE) data archive designed to provide long-term stewardship and use of data from observational, experimental, and modeling activities in the earth and environmental sciences. The ESS-DIVE infrastructure is constructed with the long-term vision of enabling broad access to and usage of the DOE sponsored data stored in the archive. It is designed as a scalable framework that incentivizes data providers to contribute well-structured, high-quality data to the archive and that enables the user community to easily build data processing, synthesis, and analysis capabilities using those data.

The key innovations in our design include: (1) application of user-experience research methods to understand the needs of users and data contributors; (2) support for early data archiving during project data QA/QC and before public release; (3) focus on implementation of data standards in collaboration with the community; (4) support for community built tools for data search, interpretation, analysis, and visualization tools; (5) data fusion database to support search of the data extracted from packages submitted and data available in partner data systems such as the Earth System Grid Federation (ESGF); and (6) support for archiving of data packages that are not to be released to the public.

ESS-DIVE data contributors will be able to archive and version their data and metadata, obtain data DOIs, search for and access ESS data and metadata via web and programmatic portals, and provide data and metadata in standardized forms. The ESS-DIVE archive and catalog will be federated with other existing catalogs, allowing cross-catalog metadata search and data exchange with existing systems. ESS-DIVE is operated by a multidisciplinary team from Berkeley Lab, the National Center for Ecological Analysis and Synthesis (NCEAS), and DataONE. The primary data copies are hosted at DOE's NERSC supercomputing facility with replicas at DataONE nodes.

Poster #BF-Hall

ESS-DIVE Publishing Life Cycle and Community Outreach

Charuleka Varadharajan[1*], Shreyas Cholia[1,2], Cory Snavely[2], Valerie Hendrix[1], Fianna O'Brien[1], Abdelrahman Elbashandy[1], Dan Gunter[1], William Riley[1], Chris Jones[3], Matt Jones[3], Amber E Budden[4], Dave Vieglais[5] and Deb Agarwal[1*]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]NERSC, Berkeley, CA
[3]NCEAS, Santa Barbara, CA
[4]DataONE, Santa Barbara, CA
[5]University of Kansas, Lawrence, KS

Contact: cvaradharajan@lbl.gov

BER Program: CESD Data Management
Project: ESS-DIVE
Project Website: http://ess-dive.lbl.gov

Wondering where to archive your DOE ESS project data? The new DOE Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) is here to help. ESS-DIVE accepts user data as "data packages," which are best described as a collection of related data files and metadata. These may be data from a sensor or a network of sensors, data from a field campaign or experiment, software for analysis or modeling, model setup and results. The current publishing life cycle involves the following steps: (1) A user wishing to submit data to the archive gathers the files to be included in a data package, and uploads them via a web portal, (2) The user specifies metadata associated with the data package, including author and citation information, as well as related references. This information can be updated at a later date, (3) The user submits the data package, and receives a system-assigned unique identifier for the data package, (4) When ready, the user shares the data publicly. The ESS-DIVE team checks the data prior to release, and a DOI is assigned. The data package becomes available for search on the ESS-DIVE data portal. The data contributor will be able to track data downloads and usage.

ESS-DIVE seeks to transform the way data from ESS research is stored and accessed by engaging the scientific research community in adopting consistent standards and protocols for data and metadata archival that improve data access. As a result, ESS-DIVE is designed to be a partnership with the scientific community, including individual DOE projects/programs, DOE cyberinfrastructure groups, and data users. The ESS-DIVE team is working to build close relationships with each of the DOE ESS projects across labs and universities with site visits, webinars and tutorials. ESS-DIVE will provide letters of support for proposers seeking to include ESS-DIVE as part of their data management plan. Additionally, ESS-DIVE is working closely with two DOE advisory groups, namely ESS-DIVE's Archive Partnership Board consisting of the leads of major ESS projects, and the ESS Cyberinfrastructure Working Groups and Executive Committee.

Poster #UF-1

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

Nancy Hess[1*]

[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA

Contact: nancy.hess@pnnl.gov

BER Program: Scientific User Facility
Project: EMSL
Project Website: http://www.emsl.pnl.gov/

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

EMSL, a DOE national user facility in Richland WA, provides integrated experimental, computational, and modeling and simulation resources and expertise for scientific studies and discovery in Earth Systems Science to users free of charge. There are numerous capability sets that are particularly relevant for such research. I) Next generation imaging and surface characterization experimental capabilities can be used to provide the spatially resolved elemental analysis, oxidation state determination, chemical speciation, mineral identification, and microbe-mineral associations necessary for understanding the chemical fate and mobility of contaminants in the biogeochemical environment or microbial communities and nutrient cycling in the rhizosphere. II) Advanced spectroscopic capabilities are used for determining the speciation of metal ions and complexes on surfaces, in solution, or incorporated into mineral phases. III) A comprehensive suite of mass spectrometry platforms for proteomics/metabolomics, whole transcriptome analysis, gene expression profiling, small RNA analysis, novel transcript identification, and many genome- and epigenome-directed applications provide EMSL users extensive capabilities for unraveling the interplay between microbes, plants, soil, and geochemistry. IV) An integrated suite of capabilities to support research in subsurface flow and transport provide data from the micron to the intermediate scale. Experts assist users with pre-experiment modeling to hydraulic characterization, numerical modeling, and post-process analysis on custom-built flowcells. V) EMSL' s Plant Ecosystem Lab offers different types of plant growth facilities including Conviron walk-in rooms and Percival chambers. This allows growing and investigating plants under environmentally controlled conditions with defined temperature, humidity, light intensity, and CO_2 levels.

EMSL is expanding capabilities to couple computational resources with data generation: we are coupling metabolomics measurements with NWChem molecular dynamics simulations to achieve "standards-free" accurate identification of metabolites thereby expanding the number and diversity of metabolites identified by mass spectrometry and we are performing genomic sequence analysis and data mining to improve the depth of coverage from proteomics studies. The extensive expertise at EMSL in multi-scale reactive transport modeling spans the pore-to-basin scale; in particular, our modeling expertise encompasses experience with a diverse suite of software systems, including SPH and TETHYS for pore- scale simulation and PFLOTRAN, Amanzi and eSTOMP for continuum-scale simulation.

Poster #UF-2

Microbial Stabilization and Destabilization of Soil Organic Carbon Across Scales

Alice Dohnalkova[1] and Petr Čapek[1]

[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA

Contact: nancy.hess@pnnl.gov

BER Program: Scientific User Facility
Project: EMSL
Project Website: http://www.emsl.pnl.gov/

EMSL provides researchers with a wide range experimental, computational, modeling and simulation approaches to investigate biogeochemical processes from molecular to ecosystem scale. In this poster we present selected approaches to study microbial stabilization and destabilization of soil organic carbon across scales.

Soil microorganisms affect the processes of soil organic carbon stabilization and destabilization at all scales of complexity, from nano- to micro- and macro-scale. At the micro-scale, we studied microbial-mineral associations in soils, where complex processes, including mineral aggregate formation, microbial mineral weathering, and soil organic matter stabilization occur. We placed in-growth mesh bags containing biotite in the ponderosa pine rhizosphere and after 9 months analyzed their contents by Fourier-transform ion cyclotron resonance mass spectrometry to obtain molecular-level identification of newly-formed organic compounds. We analyzed bacterial and fungal soil microbiomes by DNA sequencing. We used high- resolution electron microscopy to examine the nature of organo-mineral associations, aggregation, and mineral weathering processes. Weathering was validated by X-ray diffraction analysis. The results suggest that the mineral aggregation and weathering were driven by the newly formed organic matter produced by microbial activity.

At the macroscale, we used a meta-analytical approach to quantify the importance of soil microorganisms for prediction of soil organic carbon destabilization/mineralization under expected increase of temperature. We show that accounting for the size of microbial biomass in the soil improves the predictive ability of a given mathematical model by more than 500% (from 12 to 68% of explained variability in data).

Poster #UF-5

Research in Biogeochemical Sciences at the Berkeley Synchrotron Infrared Structural Biology (BSISB) Imaging Program

Hoi-Ying Holman[1], Giovanni Birarda[1,2], Liang Chen[1], Luisa Falcon[3], Christine Moissl- Eichingter[4,5], Arthur Montazeri[1], Alexander Probst[4,6], Neslihan Tas[1], and Patricia Valdespino[1]

[1]Lawrence Berkeley National laboratory, Berkeley, CA
[2]Elettra – Sincrotrone Trieste, Basovizza, Trieste, Italy
[3]Universidad Nacional Autonoma de Mexico, Mexico City, Mexico
[4]University of Regensburg, Regensburg, Germany
[5]Medical University of Graz, Graz, Austria
[6]University of Duisburg-Essen, Duisburg, Germany

Contact: hyholman@lbl.gov

BER Program: BER Genomic Science Program (GSP)
Project: SFA (Infrared Spectroscopy Imaging Program)
Project Website: https://bsisb.lbl.gov/wordpress/

The BSISB program is the only DOE/BER-funded imaging resource facility centered around special beamlines that use non-invasive but bright infrared beams to study live microorganisms and cells in terrestrial ecosystems. Since 2010, the BSISB has been developing user-driven cutting- edge infrared imaging technologies that enable researchers to acquire with chemical resolution fundamental knowledge about the nature and behavior of living microbes, microbial communities, microbe-host, and microbe-environment interactions. More than 95% of the BSISB budget goes to our Beginning-to-End (B2E) user process, which starts when a user initiates communication, safety, hands-on training, and ends when the data analysis and interpretation are completed. Throughout the B2E process, the BSISB staff communicate with the user teams to design their experiments, and to help with data analysis and interpretation if needed. The information captured is used to improve BSISB technological capabilities and align them with user needs. Here, we high-light our current capabilities and present examples of using synchrotron radiation-based Fourier Transform Infrared (SR-FTIR or sFTIR) spectral imaging techniques to study biogeochemical systems.

Poster #UF-3

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

Susannah Tringe[1*]

[1]DOE Joint Genome Institute, Lawrence Berkeley National Laboratory, Walnut Creek, CA

Contact: sgtringe@lbl.gov

BER Program: Scientific User Facility
Project: JGI
Project Website: http://www.jgi.doe.gov

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, particularly in the molecular microbial ecology of diverse terrestrial environments, and continues to evolve as a state-of-the-art genomic science user facility.

Poster #UF-6

The DOE Atmospheric Radiation Measurement (ARM) Climate Research Facility

Sally McFarlane[1*]

[1]Office of Biological and Environmental Research, Office of Science, DOE, Washington, DC

Contact: sally.mcfarlane@science.doe.gov

BER Program: Scientific User Facility
Project: ARM
Project Website: http://www.arm.gov

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 #UF-4

DOE Synchrotron* Capabilities and Structural Biology Resources for Environmental Research**
*Supported by DOE Basic Energy Sciences (BES)
**Supported by DOE Biological and Environmental Research (BER)

John Bargar[1], Ken Kemner[2], Peter Nico[3], Amy Swain[4], and Ryan Tappero[5]

[1]SLAC National Accelerator Laboratory
[2]Argonne National Laboratory
[3]Lawrence Berkeley National Laboratory
[4]Office of Biological and Environmental Research, DOE
[5]Brookhaven National Laboratory

Contact: bargar@slac.stanford.edu, Amy.Swain@science.doe.gov
BER Program: Subsurface Biogeochemistry Research and Structural Biology Infrastructure
Websites: http://BERStructuralBioPortal.org

The DOE BER Environmental System Science programs seeks to advance a robust predictive understanding of terrestrial surface and subsurface ecosystems, within a domain that extends from the bedrock to the top of the vegetated canopy and from molecular to global scales. This activity focuses on understanding the interdependencies involving biogeochemical, genomic, ecological, geohydrological, and migration processes involving nutrients and contaminants, diverse landscape systems, and spanning arctic to tropical climates.

Deep understanding at a molecular scale of environmental systems within the terrestrial ecosystem and subsurface research programs requires structure and function studies of system components, which include biological behavior, abiotic-biotic interactions, and molecular transformations that control the mobility of contaminants, nutrients, and critical vegetative and biogeochemical elements.
DOE supports a wide array of synchrotron- and neutron- based techniques for characterizing structure, function and interrelationships among complex molecular components that are relevant to these systems. The spatial and temporal resolutions available from neutron and photon beams enable characterization and imaging of system components and interactions among plants, microbes and minerals. Accessible scales range from subnanometer to centimeter length and over time dimensions from femtoseconds to seconds.

Structural insights at the atomic, molecular and mesoscale level are critical for developing multi-scale, multi-component models that can be used to predict system behaviors. These insights advance the goals of the terrestrial ecosystem program to understand the role of ecosystems in climate, and the subsurface biogeochemical program that pursues a predictive understanding of how watersheds function as complex hydrobiogeochemical systems.

Two posters will present the BES-supported synchrotron capabilities for environmental system science and the BER-supported resources at synchrotron and neutron facilities for biological investigations relevant to environmental systems.

Poster #UF-7

KBase: An Integrated Systems Biology Knowledgebase for Predictive Biological and Environmental Research

Adam P. Arkin[1], Robert Cottingham*[3], Chris Henry[2], Nomi Harris[1], Ben Allen[3], Jason Baumohl[1], Shane Canon[1], Stephen Chan[1], John-Marc Chandonia[1], Dylan Chivian[1], Paramvir Dehal[1], Meghan Drake[3], Janaka Edirisinghe[2], Jose Faria[2], Uma Ganapathy[4], Annette Greiner[1], Tian Gu[2], James Jeffryes[2], Marcin Joachimiak[1], Roy Kamimura[1], Keith Keller[1], Vivek Kumar[5], Sunita Kumari[5], Miriam Land[3], Sean McCorkle[4], Arman Mikaili[2], Dan Murphy-Olson[2], Arfath Pasha[4], Erik Pearson[1], Gavin Price[1], Priya Ranjan[3], William Riehl[1], Samuel Seaver[2], Alan Seleman[2], James Thomason[5], Doreen Ware[5], Shinjae Yoo[4], Qizhi Zhang[2], Diane Zheng[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA
[2]Argonne National Laboratory, Argonne, IL
[3]Oak Ridge National Laboratory, Oak Ridge, TN
[4] Brookhaven National Laboratory, Upton, NY
[5]Cold Spring Harbor Laboratory, Cold Spring Harbor, NY

Contact: cottinghamrw@ornl.gov
BER Program: BER
Websites: http://kbase.us

Project Goals: The DOE Systems Biology Knowledgebase (KBase) is a free, open-source software and data platform that enables researchers to collaboratively generate, test, compare, and share hypotheses about biological functions; analyze their own data along with public and collaborator data; and combine experimental evidence and conclusions to model plant and microbial physiology and community dynamics. KBase's analytical capabilities currently include (meta)genome assembly, annotation, comparative genomics, transcriptomics, and metabolic modeling. Its web-based user interface supports building, sharing, and publishing reproducible, annotated analysis workflows with integrated data. Additionally, KBase has a software development kit that enables the community to add functionality to the system.

The U.S. Department of Energy (DOE) has invested substantially in environmental and biological system science research to investigate the complex interplay between biological and abiotic processes that influence soil, water, and environmental dynamics of our biosphere. The community that has grown around these efforts has recognized the need to lower the barrier to accessing computational tools, data, and results, and to work collaboratively to accelerate the pace of their research. The DOE Systems Biology Knowledgebase (KBase, kbase.us) is a software platform designed to provide these needed capabilities.

KBase currently has over 160 analysis tools (see https://narrative.kbase.us/#appcatalog) that offer diverse scientific functionality for (meta)genome assembly, contig binning, genome annotation, sequence homology analysis, tree building, comparative genomics, metabolic modeling, community modeling, gap-filling, RNA-seq processing, and expression analysis (see Figure 1). Users can build and share sophisticated workflows by chaining together multiple apps–for example, one could predict species interactions from metagenomic data by assembling raw reads, binning assembled contigs by species, annotating genomes, aligning RNA-seq reads, and reconstructing and analyzing individual and community metabolic models.

Computational experiments in KBase are saved in the form of *Narratives*. A finished Narrative represents a complete record of everything the authors did to complete their analysis. This recording of a user's KBase activities within a sharable Narrative is a central pillar of KBase's support for reproducible transparent research, simplifying the re-purposing, re-application, and extension of scientific techniques.

Small Business Innovative Research (SBIR) Awards

Poster #21-41

Microbial Sensor for Characterizing and Monitoring Watersheds and Terrestrial Environments Including the Rhizosphere

Scott Burge[1*]

[1]Burge Environmental, Inc., Tempe AZ

Contact: Scott@burgenv.com

BER Program: SBR
Project: SBIR
Project Website: https://www.burgenv.com/

The microbial sensor is an electrochemical sensor measuring the electrical potential generated by microbial communities populating the surface of the probes. The system determines the redox potential and/or dissolved oxygen concentrations of aquatic and terrestrial environments. System instrumentation consists of electrochemical sensors (a cathode and several anodes) and a signal acquisition/communication module. The automated system collects (typically every .5 hour) and transmits data to a web site for visualization and other data reduction methodologies. The sensor system requires no maintenance and sensors have been deployed in sediments for over 900 days with no significant degradation of the signals. Over ten systems are currently deployed in aqueous environments including contaminated aquifers, wastewater treatment facilities, fish farms and algae research operations. Based on the unique characteristics of the electrochemical components, the system can operate in terrestrial environments including the rhizosphere. We will present investigations of both aquatic (laboratory and field) and terrestrial (laboratory) environments.

Poster #9-1

High Speed VNIR/SWIR Hyperspectral Imager for Quantifying Terrestrial Ecosystems

Julia R. Dupuis[1*], David J. Mansur[1], Joy Stafford[1], and Jonathan Rameau[1]

[1]Physical Sciences, Inc., Andover, MA

Contact: jdupuis@psicorp.com

BER Program: TES
Project: SBIR
Project Website: http://www.psicorp.com/

Physical Sciences Inc. (PSI) is developing a high-speed visible/near infrared, shortwave infrared (VNIR/SWIR) hyperspectral imaging (HSI) sensor for airborne, dynamic, spatially-resolved vegetation trait measurements to support advanced terrestrial modeling. This technology aligns with DoE's requirements for broad spectral range hyperspectroscopic instrumentation in a compact form factor suitable for deployment on a small, rotary wing unmanned aircraft system (UAS). The VNIR/SWIR-HSI sensor employs a digital micromirror device as an agile, programmable entrance slit into VNIR (500-1000 nm) and SWIR (1200-2500 nm) grating spectrometer channels, each with two-dimensional focal plane arrays. The sensor acquires 360 spectral bands over a 30º field of view (FOV) in 2.5 s. The architecture enables staring mode hyperspectral imaging and does not require constant aircraft motion to acquire the data cube, making it compatible with a hovering, rotary wing UAS. The data product is a stream of high quality, calibrated, orthorectified spectral reflectivity cubes which are stitched together for subsequent analysis over a wide area. The capability includes spectral matching algorithms based on a linear discriminant analysis for vegetation species mapping.

The design and build of the VNIR/SWIR HSI sensor is presented with emphasis on laboratory and rooftop/tower testing of local vegetation. Performance including spectral resolution and accuracy across the full spectral range and noise equivalent reflectivity across the FOV is reported. The 14.5 lb sensor package is presently being integrated to a Free Fly Alta8 UAS for flight testing, the preliminary results from which are included. Future upgrade plans are discussed.

Poster #21-40

Dissolved Oxygen Sensor System for Real-time, In-situ Subsurface Monitoring of the East River Hyporheic Zone in Crested Butte, CO

Ruby Ghosh[1*], Dean Shooltz[1], Michael Freeman[1], Bruce Bright[1], Kenneth Williams[2], Michelle Newcomer[2], and Michael Williams[3]

[1]Opti O2, Okemos, MI
[2]Lawrence Berkeley National Laboratory, Berkeley, CA
[3]Ohio State University, Columbus, OH

Contact: ghosh@optio2.com

BER Program: SBIR
Project: SBIR
Project Website: www.optio2.com

Environmental sensor systems for subsurface dissolved oxygen (DO) concentration measurement are of interest because of the outsized role DO plays in catalyzing a diversity of environmentally important biogeochemical reactions. Commercially available DO sensors cannot provide the desired spatial and temporal density for resolving data over extended periods at the 'ecosystem level'. We have developed an optical oxygen sensing technoloty to monitor oxygen concentrations in flowing water, as well as both fully saturated and unsaturated soil with the same sensor.

We have established a remote sensing station at the DOE, East River, SFA in Crested Butte, CO. This station is solar/battery powered to autonomously transmit data from an array of probes deployed in the meander. These include three Opti O2 DO probes that are buried directly under the stream bed at depths of 10cm, 20cm and 35 cm and a fourth probe within the river stream itself. We have been collecting data from all four probes continuously over the last six months, including under winter conditions, at a data rate of one measurement every 5 minutes. The data stream is comprised of eight simultaneous channels, dissolved oxygen and temperature of the river water and the three location under the river bed itself. Our objective is to demonstrate a monitoring technology that provides insight into spatial and temporal variations in dissolved oxygen as a result of hydrological factors, such as seasonal infiltration events and excursions groundwater elevation.

Poster #21-39

Monitoring Sediment Oxygen Demand in a Coastal Ecosystem with a Robust, In-situ Oxygen Probe

Ruby N. Ghosh[1*], Dean Shooltz[1], Terry Ball[1], Michael Freeman[1], Gary Gill[2], Jay Grate[2] and Stanley Tomich[2]

[1]Opti O2, Okemos, MI
[2]Pacific Northwest National Laboratory, Richland, WA

Contact: ghosh@optio2.com

BER Program: SBIR
Project: SBIR
Project Website: www.optio2.com

An important parameter in modeling the biogeochemistry of coastal ecosystems is the ability to monitor in real-time sediment oxygen demand. The need for data over a wide range of time and length scales necessitates a dissolved oxygen (DO) sensor technology that is simultaneously robust and cost/resource effective. We report on the development of a benthic flux chamber equipped with a compact, self-contained DO probe designed to withstand the rigors of the marine environment over extended periods of time. This autonomous oxygen probe is cost effective and labor efficient to enable temporally resolved measurements of sediment oxygen demand at multiple locations during weather events or marine cycles of interest. We are working to understand coastal eutrophication and hypoxia events of the Sequim Bay Watershed, WA, USA.

We monitor biological oxygen demand in the sub tidal sediments of the Puget Sound with a benthic flux chamber containing the Opti O2 dissolved oxygen probe and data recording module. DO concentration is determined by measuring the oxygen quenching of the phosphorescence from metal-halide optical indicators. The sensor probe is completely self- contained within a compact water proof body which includes both the optical sensing film and the miniature fluorescence spectrometer. The low power requirements of the spectrometer and data logging module enables a single 9V alkaline battery to power the system for at least 750 hours, collecting one data point every 5 minutes. We will demonstrate that our DO probe can accurately monitor DO in both saline and fresh water with the same instrumentation, i.e. without the need for recalibration under changing water conditions as well as the ability of the probe to withstand the corrosive nature of a tidal coastal environment.

Our technology is well suited for long term studies of carbon cycling at the dynamic interface between coastal and terrestrial environments such as the Olympic peninsula.

Poster #21-42

Analytical Instrumentation for *in-situ* Biogeochemical Research

Donald Nuzzio[1*]

[1]Analytical Instrument Systems, Inc., Flemington, N.J.

Contact: ais@aishome.com

BER Program: SBR
Project: SBIR

In order to fully understand biogeochemical reactions that affect any environment, the utilization of in-situ analytical tools are key to understanding the chemistry of these complex systems. Bringing analytical instruments into the field that have been traditionally left in the lab, will offer a clearer picture of biogeochemical reactions in real time. Traditionally samples are taken from the field and later analyzed in a lab where the context of the sample may have been compromised.

This SBIR Phase II project is focused on building a new type of electrochemical device that is capable of collecting data from any environment on Earth. These new systems are voltammetric in nature and will allow the determination of the standard biogeochemicals in-situ including and not limited to, oxygen, sulfide, iron, iron sulfide, and manganese directly on one sensor in real time in about 3-5 seconds. These new instruments are capable of analyzing any ion in the environment including mercury to heavy metals from acid mine drainage down to the parts per trillion level. Several versions of this instrument are being developed for particular applications that have specific needs. A hand-held unit is being developed to quickly ascertain a particular site of interest that will allow the user to make a judgment on deploying the long-term unit for monitoring diurnal cycling of pertinent biogeochemical over time. The main deployable unit will be used to collect data over time and allow that data to be gathered and transmitted directly to a cloud server system. What makes these systems unique are the low power electronics and the new electrode systems that can be deployed for many months to years with little user servicing. We are currently going to deploy some of these new systems at the Crested Butte area in Colorado with Kenneth Williams and in Oak Ridge Tennessee with Scott Brooks.

Other devices that are produced by Analytical Instrument Systems, Inc. (AIS) include a DLK-MO-1 micro-observatory that allows data collection from a wide assortment of sensors that can be obtained commercially, an in-situ combination electrochemical analyzer and an HPLC (AIS ISEA-HPLC) instrument that allows for the determination of all the standard biogeochemical analytes, anions and organics. These systems use an embedded web server and can be addressed through standard Ethernet with any web browser. One of these instruments is being used to analyze red tide in Florida at Mote Marine Institute.

In summary AIS has had direct experience of analyzing some of the most extreme environments on Earth. From hydrothermal vents on the ocean floor at 9N EPR aboard the Alvin DSV to geysers in Yellowstone and Iceland to acid mine drainage from the most naturally polluted river on Earth, the Rio Tinto in Spain.

Poster #9-3

HDTomoGPR: Ground Penetrating Radar System and Algorithms for Fine Root Analysis

Gerald Sabin,[1*] Jamar Robinson,[1] Michael Wicks,[2] Andrew Bogel,[2] and Nihad Alfalsaye,[2]

[1]RNET Technologies, 240 West Elmwood Drive, Dayton, OH 45459;
[2]University of Dayton, 300 College Park, Dayton, OH 45469

Contact: gsabin@RNET-Tech.com

BER Program: SBIR
Project: SBIR

The HDTomoGPR is a mobile, field-deployable high-resolution subsurface 3D data collection platform for below ground imaging. The system can be used in any situation where an accurate underground visualization is required. Potential use cases include fine-grained root analysis, concrete analysis, archeology, and geological survey of construction sites. The primary benefits, as compared to other GPR systems, are improved resolution and improved 3D images for easy survey analysis. The 3D imaging benefits are derived from the increased data collection (via multiple antenna look angles collected from a stable data collection platform) that supports state-of-the-art GPR tomography to generate high-resolution images.

HDTomoGPR utilizes novel radar processing technology of data from an unconventional radar platform using COTS RF and compute technology. The HDTomoGPR radar system operates from 1GHz to 12 GHz and utilizes an Ultra-Wide Band (UWB) radar and data processing suite to balance resolution and penetration depth. The high frequency bands provide superior resolution at shallow depths of penetration, while the lower frequency bands allow greater subsurface penetration. The system uses a nonlinear stepped FM (frequency modulated) signal, and is designed to compensate for the frequency selective and site specific attenuation exhibited by soil and rock formations.

In order to increase the resolution and generate high quality 3D images, HDTomoGPR processes the phase measurement data tomographically (i.e., from a variety of viewing angles, e.g. geometric diversity). The data is then adaptively combined coherently to produce the high-resolution 3D image. A major advantage of this novel adaptive tomographic signal/image processing techniques is that the target is viewed from multiple look directions, which overcomes the effect of dominant scattering (strong reflections) from the front surfaces (leading edges) of the target and subsequent shadowing (weak reflections) of the back surfaces of targets. In addition, the resolution of the target image is enhanced as a result of multi-static tomographic signal processing. The computed images can achieve the Rayleigh resolution limit of $\lambda/3$.

In order to collect data over a variety of look angles (i.e., GPR antenna positions), the trailer includes a 1000mm by 1200mm scanning platform and houses a precision antenna placement system, RF equipment (1 to 12 GHz scan capabilities using a stepped FM waveform), and a compute platform. A prototype HDTomoGPR scanner has been developed, fabricated and deployed. Experimental results to date include indoor laboratory experiments and outdoor tests with a commercial agricultural partner.

Poster #9-2

A Compact, Broad-Band Hyperspectral SpectroRadiometer

Rand Swanson[1]

[1]Resonon, Bozeman, MT

Contact: swanson@resonon.com

BER Program: TES
Project: SBIR
Project Website: www.resonon.com

Progress on a compact, broad-band (350-2,500 nm) hyperspectral imager for UAV deployment is presented. The novel optical design provides an additional degree of engineering freedom as compared to conventional push-broom imaging spectrometers. This additional degree of freedom is used to obtain high throughput with near AVIRIS-like Signal-to-Noise performance expected.

Poster #21-64

Predictive Assimilation Framework: Cloud based System for Site Monitoring

Roelof Versteeg[1*]

[1]Subsurface Insights, Hanover, NH

Contact: roelof.versteeg@subsurfaceinsights.com

BER Program: SBR
Project: SBIR
Project Website: http://www.subsurfaceinsights.com/paf

Over the past several years Subsurface Insights (under SBIR funding) has developed PAF (Predictive Assimilation Framework), a cloud based multi tenant web application for site monitoring and understanding. From its inception PAF has been designed as a vertically integrated system which should translate subsurface data into actionable information in an auditable, automated and low friction manner.

To achieve this PAF is implemented as a cloud based software application with five components: (1) data acquisition, (2) data management, (3) data assimilation and processing, (4) visualization and result delivery and (5) workflow orchestration. PAF is provided as software as a service (SAAS) with modular functionality. This functionality can be activated based on available data or project needs. The main organizational unit in PAF is a project. Projects have users (with different levels of privileges). Users can be members of multiple projects and can easily switch between projects through both the mobile and browser interface. All projects share the same database models and information architecture, but for security, efficiency and portability reasons each project has its own database.

PAF is implemented serverside using ZF2 (Zend Framework 2), a modular PHP web application framework and python. Rich front end functionality is provided by Javascript and CSS and back end processing is implemented in python workflows.

Projects are implemented in software through dynamic routing. PAF also supports the use of domain aliases (e.g. https://weatherstations.rmbl.org is a PAF site, even though it looks to be hosted at rmbl.org). All PAF capabilities are exposed through APIs. PAF is integrated with a variety of numerical models including PFLOTRAN, Landlab and E4D. PAF can ingest a broad range of data including timelapse geophysical data from electrical resistivity and DTS systems, time series sensor data from a broad number of physical sensor data, geochemical data and remote sensed data. PAFs modular design, API centric software architecture, hierarchical user model and customizability has proven to be very well suited to meet a number of different demands. Users interact with PAF through either a standard web browser or the mobile app “Site Info” (available for IOS and Android). PAF is currently used in about 20 projects and is seeing increased acceptance in the private sector, including for agricultural and water resource applications.

We will discuss the overall PAF architecture, design choices, API interface and several use cases and recent enhancements and lay out our plans for future enhancements of PAF.