2020

ENVIRONMENTAL SYSTEM SCIENCE (ESS) VIRTUAL PRINCIPAL INVESTIGATORS MEETING

ABSTRACT BOOK

May 19-20, 2020

2020 Environmental System Science (ES) Virtual Principal Investigators Meeting

May 19-20, 2020

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: Mr. Paul Bayer (paul.bayer@science.doe.gov)
Dr. Jennifer Arrigo (Jennifer.arrigo@science.doe.gov)
Dr. Amy Swain (amy.swain@science.doe.gov)

Program Website: www.doesbr.org/

Table of Contents

(Click on any line to advance to the abstract)

Environmental System Science

Student Abstracts

Seasonal Shifts in Mineral and Metabolic Constraints Regulate Carbon Export from Floodplain Soils

Carolyn Anderson[1]*, Christian Dewey[2], Malak Tfaily[3], Ravi Kukkadapu[4], William Kew[4], Peter Nico[5], Patricia Fox[5], Scott Fendorf[2], Marco Keiluweit[1]

[1]University of Massachusetts Amherst, Amherst, MA
[2]Stanford University, Stanford, CA
[3]University of Arizona, Tuscon, AZ
[4]Pacific Northwest National Laboratory, Richland, WA
[5]Lawrence Berkeley National Laboratory, Berkeley, CA

(cganderson@umass.edu)

Project Lead Principal Investigator (PI): Scott Fendorf

BER Program: SBR

Project: University Project

Floodplain soils are large and dynamic reservoirs of carbon (C), where seasonal flooding regulates both C storage and downstream water quality. Timing and frequency of seasonal flooding events are altered by climate change, increasingly subjecting floodplain soils to extreme flooding or droughts. These changes may have profound implications for greenhouse gas emissions or dissolved organic carbon (DOC) export from floodplain soils. Yet, the underlying (hydro)biogeochemical controls on C retention and export in floodplain soils are poorly constrained, limiting our ability to predict responses to climate change. Here we aimed to determine how seasonal flooding, and associated variations in redox conditions, impact the dominant controls on microbial C cycling in floodplain soils. Using in-field monitoring with advanced analytical and molecular tools, we examined how changes in mineral interactions and microbial activity during flooding and subsequent drainage affected C export from floodplain soils of the mountainous East River watershed (Gothic, Colorado). Our results show that reduced conditions during flooded periods caused reductive dissolution of Fe (hydr)oxide, mobilizing previously sorbed organic matter and enhancing DOC export. At the same time, flooding decreased CO_2 production and selectively preserved chemically reduced organic matter, likely due to metabolic constraints on microbial respiration. Upon drainage and re-oxygenation of floodplain soils, however, CO_2 production increased, partly due to the oxidation of reduced organic compounds, but was limited by the concurrent entrapment of DOC by newly precipitated Fe (hydr)oxides. Combined, our results reveal that temporal variations in redox conditions during seasonal flooding shift the relative and interactive effects of mineral and metabolic constraints on CO_2 and DOC export from floodplain soils. Implications of these findings for floodplain C vulnerability to future changes in timing, intensity and duration of flooding events will be discussed.

Title: **Seeking the best-fit microbial-relevant parameters via model calibrations: site-specific single dataset or cross-site multiple datasets?**

Siyang Jian[1*], Jianwei Li[1], Gangsheng Wang[2,3], Laurel A. Kluber[4], Christopher W. Schadt[4] and Melanie A. Mayes[2]

[1] Department of Agricultural and Environmental Sciences, Tennessee State University, Nashville, TN 37209, USA
[2] Environmental Division & Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA
[3] Institute for Environmental Genomics and Department of Microbiology & Plant Biology, University of Oklahoma, Norman, Oklahoma, 73019, USA
[4] Biosciences Division & Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

Contact: sjian@my.tnstate.edu, jli2@tnstate.edu, mayesma@ornl.gov

Project Lead Principle Investigator (PI): Dr. Paul Hanson
BER Program: TES
Project: Student travel award
Project Website: https://tes-sfa.ornl.gov/

Project Abstract:
Soil organic carbon (SOC) is a significant component of the global carbon cycle, but model projections of SOC display large uncertainty in response to future climate change. Integrating microbial community dynamics into models potentially improves the accuracy of SOC projection, yet there are challenges on how to achieve the best-fit microbial parameters for various soil and ecosystem types. Based on a long-term (729 days) soil incubation dataset with soils collected from forest and grassland sites covering four soil orders, we obtained microbial parameters for the Microbial-ENzyme Decomposition (MEND) model using either single-case calibration (SCC) or by grouping the datasets according to soil type (i.e. multiple-case calibration or MCC). Additionally, we calibrate decay constants of a first-order model modified from the MEND using multiple-case dataset to compare behavior of traditional model with microbial model. The SCC calibration showed that model performance increased as more measurements were integrated into calibration. But combining measurements across other sites or ecosystems using MCC produced less satisfactory model performance compared to the SCC. First-order model also had worse performance when cases number increased. Our results indicate that parameterization of the MEND model is highly site-specific and microbial models may be more computationally- and data-intensive compared to traditional modeling approaches.

Microbial diversity drives specialization in litter decomposition and metabolic products

Nanette C. Raczka[1]*, Juan P. Nevado[2], Ember M. Morrissey[2], Zachary B. Freedman[2] and Edward R. Brzostek[1]

[1]Department of Biology, West Virginia University, Morgantown, WV;
[2]Division of Plant and Soil Sciences, West Virginia University, Morgantown, WV

(ncr0008@mix.wvu.edu)

Project Lead Principle Investigator (PI): Edward R. Brzostek BER
Program: TES
Project: University project

Soil C formation and loss is controlled by the chemical complexity of substrate inputs and the ability of microbes to efficiently use those substrates to drive growth and decomposition.
Litterbag studies infer that microbes exposed to a wide range of substrate complexity have greater functional diversity in their decomposition pathways than microbes exposed to only simple substrates. Here, we test this theory using DNA stable isotopic probing and metabolomics to quantitatively measure the fate of litters that vary in complexity into microbial biomass and metabolic products. We used trees that differ in mycorrhizal association, ectomycorrhizal (ECM) vs. arbuscular mycorrhizal (AM), as a model system to investigate the extent to which litter complexity and microbial community composition influence microbial product formation. We hypothesized that high quality AM litter would enhance microbial metabolism to a greater extent than low quality ECM litter. Further, we predicted that due to microbial specialization in ECM soils, decomposition of either litter type would be faster than AM soils. To test these hypotheses, we incubated isotopically labeled ^{13}C AM (tulip poplar, *Liriodendron tulipifera*) and ECM (red oak, *Quercus rubra*) litter in soils from AM and ECM dominated plots in a 100-year- old forest in West Virginia. In contrast to our hypotheses, we found evidence that different microbial groups favor AM vs ECM litter in AM soils leading to divergent decomposition products. Fungi and bacteria decomposing either litter type in AM soils were different and more diverse than microbes in the ECM soils. While overall, fungi incorporated more litter into biomass than bacteria, AM soil fungal communities that decomposed AM litter were distinct from those that decomposed ECM litter. This variable preference for litter shifted the metabolic pathways that were used and produced distinctly different microbial products. In contrast to the AM soils, ECM soil microbes were not flexible in utilizing the added litter substrate, nor did the resulting metabolic products differ with litter type. This may be driven by lower diversity in fungal and bacterial communities in the ECM soils. Moreover, ECM soil communities exhibited little distinction in the type of litter incorporated into biomass, resulting in a single metabolic pathway that produced comparable microbial products. These results challenge our understanding of microbial control on decomposition and suggest that microbial diversity drives substrate use.

Title: **The response of greenhouse gas production (GHG) pathways to elevated temperature in the SPRUCE peatland**

Tianze Song[1*], Max Kolton[1], Jose Rolando[1], Yutong Liu[1], Rachel Wilson[2], Jason Keller[3], Scott Bridgham[4], Jeff Chanton[2], and Joel E. Kostka[1]

[1]Georgia Institute of Technology, Atlanta, GA;
[2]Florida State University, Tallahassee, FL;
[3]Chapman University, Orange, CA; and [4] University of Oregon, Eugene, OR

Contact: joel.kostka@biology.gatech.edu
Project Lead Principle Investigator (PI): Joel E. Kostka

BER Program: TES

Project: University project

Project Website: Affiliated with SPRUCE; https://mnspruce.ornl.gov/

Project Abstract: GHG emission from peatlands is hypothesized to increase in response to warming from climate change. Although methanogenesis is considered as the dominant terminal electron accepting process (TEAP) coupled to organic matter degradation, the ratio of GHGs (CO_2:CH_4) emitted from these wetlands often does not match with predicted stoichiometry. The objectives of this study are to validate field observations and modeling efforts through understanding the mechanisms and controls of GHG production in the SPRUCE peatland. Over the past 4 years, GHG production rates were quantified in microcosm experiments with fresh peat and porewater collected from the S1 bog of the Marcell Experimental Forest in parallel with field observations. Microcosm treatments included porewater alone, porewater plus peat, a range of temperatures (4 to 25 ℃), and amendment with potential electron acceptors/ donors.
Warming resulted in a substantial increase in CH_4 and CO_2 production rates and a decline in CO_2:CH_4 ratio. Acetate accumulated in treatments at near in situ temperature (4 ℃), indicating a threshold at which acetogenesis outcompetes methanogenesis. In contrast, although hydrogenotrophic methanogens show a higher relative abundance in field observations, acetoclastic methanogenesis predominates, with methane production becoming more hydrogenotrophic with warming as indicated by stable isotope data. Lower CO_2:CH_4 ratios were found at the onset of incubations and with DI water in comparison to porewater, suggesting that organic electron acceptors in the porewater suppress methane production under in situ conditions. Amendment with potent electron acceptors (e.g. nitrate) stimulate a large increase in CO_2 production and a suppression in methane production, pointing to electron acceptor limitation. Overall, the results corroborate field data to indicate that GHG production will increase and become more methanogenic with warming in SPRUCE soils. This is troubling since the sustained-flux global warming potential of CH_4 is now estimated at 45-times greater than that of CO_2 on a 100 y timescale.

Title: **Carbon Dioxide Production in Bedrock beneath Soils Substantially Contributes to Forest Carbon Cycling**

Alison K. Tune,[1*] Jennifer L. Druhan,[2] Jia Wang,[2] Philip C. Bennett,[1] Daniella M. Rempe[1]

[1] The University of Texas at Austin, Austin, TX;
[2] The University of Illinois Urbana-Champaign, Urbana, IL;

Contact: (alisontune@utexas.edu)

Project Lead Principle Investigator (PI): Dr. Jennifer Druhan

BER Program: SBR

Project: A radioisotope – enabled reactive transport model for deep vadose zone carbon (DE-SC0019198), University Project

Project Website: None

Project Abstract:

Soils are widely considered the primary terrestrial organic matter pool mediating carbon transactions with the atmosphere and groundwater. However, in many terrestrial environments, roots and the associated microbial communities extend below soils and into fractured bedrock. While it is likely that this extension of the rooting zone alters the hydrologic and biogeochemical dynamics of the ecosystem, it is not known if these dynamics have a significant impact on carbon cycling within and from the subsurface. Here we show substantial production of CO_2 in weathered bedrock at 4-8m below the thin soils (<0.5 m thick) of a Northern California forest using innovative monitoring technology for sampling gases and water in fractured rock. The deep CO_2 production supports a persistent upward flux of $CO_{2(g)}$ year round from bedrock to soil, constituting up to 29% of the average daily CO_2 efflux from the land surface. When water is rapidly traversing the fractured bedrock vadose zone, nearly 50% of the CO_2 produced in the bedrock dissolves into water, promoting water-rock interaction and export of dissolved inorganic carbon (DIC) from the unsaturated zone to groundwater, constituting as much as 80% of the DIC exiting the hillslope. These results indicate we should consider carbon cycling within weathered and fractured rock in larger climate and ecosystem models as a source of CO_2 to the atmosphere, groundwater, and streamwater.

Hydraulic responses of *Cornus drummondii* to fire frequency and drought in a tallgrass prairie

Kimberly O'Keefe[1], Kevin Wilcox[2]*, Jesse Nippert[3], Rachel Keen[3], Lydia Zeglin[3], and Katherine McCulloh[1]
[1]University of Wisconsin-Madison, Madison, WI;
[2]University of Wyoming, Laramie, WY;
[3]Kansas State University, Manhattan, KS

(okeefe4@wisc.edu)

Project Lead Principal Investigator (PI): Jesse Nippert
BER Program: TES
Project: University project

The increase in abundance and density of woody plants in herbaceous ecosystems (i.e., woody encroachment) is occurring globally and is driven by reduced fire frequency, climate change, and the utilization of deeper, more reliable soil water by woody plants. Thus, a comprehensive understanding of the physiological processes through which woody plants use deep water, particularly in response to different fire and climate regimes, will provide greater insight into the dynamics and consequences of woody encroachment. Our objective was to assess how experimental changes in water availability and fire frequency impact water-use traits in *Cornus drummondii*, the primary encroaching shrub within North American tallgrass prairies. Rainout shelters that either reduce precipitation by 50% (drought) or 0% (control) were built over mature shrubs growing in sites that are burned at 1-year and 4-year frequencies. We assessed the water transport capability of shrubs growing in each water*fire treatment by measuring the maximum hydraulic conductance (K_{max}) of entire root systems, stems, and leaves. We also assessed the vulnerability of stems and roots to loss of function caused by water stress by measuring vulnerability curves and calculating the pressure at which 50% of the maximum hydraulic conductivity is lost (P_{50}). Roots exhibited the greatest K_{max} (0.14 ± 0.01, 0.09 ± 0.003, and 0.06 ± 0.003 kg^1 s^{-1} m^{-2} MPa^1 in roots, stems, and leaves, respectively) but were also the most vulnerable to water stress (P_{50}=-0.64 ± 0.24 and -3.95 ± 0.35 MPa in roots and stems). Root K_{max} was lower in 1-year burned shrubs exposed to drought compared to 1-year burned control shrubs (0.08 ± 0.01 vs 0.19 ± 0.04 kg^1 s^{-1} m^{-2} MPa^1), but root vulnerability did not differ among water*fire treatments. Conversely, stem K_{max} did not differ among treatments, but 1-year burned stems were more vulnerable to water stress than 4-year burned stems, particularly when exposed to drought (P_{50}=-3.19 and -4.87 MPa for 1- and 4-year burned drought stems). Thus, frequent burning reduced root transport capability and concomitantly increased the vulnerability of stems to water stress, but only under drier conditions. Future work will investigate whether these responses to frequent burning and drought are associated with reduced shrub growth under future climate scenarios.

Environmental System Science

Early Career Awards

Microbial environmental feedbacks and the evolution of soil organic matter

Stephany Chacon[1], Aizah Khurram[1], Hoi-Ying Holman[2], Liang Chen[2], Lee Dietrich[3], Daniela Cusack[3], **Nicholas J Bouskill[1]**
[1]Climate and Ecosystem Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720.

[2]Berkeley Synchrotron Infrared Structural Biology Program, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720.

[3]Department of Ecosystem Science and Sustainability, Colorado State University, Fort Collins, CO, 80523.

The vast majority of Earth's organic matter is stored in soil. The products of microbial metabolism as well as dead microbes (necromass), along with residues from plants and other organisms at different stages of decomposition, constitute a large fraction of that soil organic matter (SOM). The ability of microbes to modify and degrade SOM depends on physicochemical characteristics of the soil, affecting SOM stability and persistence.
While the contributions of microbes to the decomposition and loss of SOM have been intensively studied, their role in maintaining terrestrial SOM is poorly understood.
Specifically, how fungi, bacteria, and archaea participate in SOM production, its interaction with minerals, and the formation of soil aggregates remains a significant gap in our understanding of the terrestrial carbon cycle. Herein, we employ field and laboratory experiments to further understand the role of microbial communities in stabilizing SOM under drought and fluctuating wet-dry cycles in clay-rich tropical soils. We begin by identifying traits characteristic of the single cell physiological response to drought stress through real-time and non-destructive Fourier-transform infrared spectroscopy at the Advanced Light Source at LBNL. This dataset serves as a baseline for the interpretation of molecular data generated across several different scales in complexity, beginning with simple community responses to drought within an abstraction of the soil environment. We scale up through a mesocosm experiment with intact soil cores collected from Isla Buena Vista, a kaolinite rich soil within a tropical rainforest, which also serves as the location of a long-term drying experiment (termed *Parched.Panama*), that serves as the final experimental scale. We use a combination of metagenomic sequencing and metabolomic profiling to examine how traits expressed within the laboratory and field experiments feedback on to the composition of soil organic matter. These three interacting scales will be used to parameterize and benchmark a mechanistic model coupling above- and belowground processes (the *ecosys* model), to predict the fate of SOM on longer time scales.

Department of Energy Early Career Research Program Grants to N.J. Bouskill, #FP00005182 and D.F. Cusack #DE-SC0015898. This research used resources of the Berkeley Synchrotron Infrared Structural BioImaging (BSISB) Program at the Advanced Light Source, which is a DOE Office of Science User Facility under contract no. DE-AC02-05CH11231.

Cell Wall *O*-Acetyl and Methyl Esterification Patterns of Leaves Reflected in Atmospheric Emission Signatures of Acetic Acid and Methanol

Rebecca A. Dewhirst[1], Cassandra A. Afseth[1], Cristina Castanha[1], Jenny C. Mortimer[2,3], and Kolby J. Jardine*[1]
[1]Climate and Ecosystem Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA; [2]Joint BioEnergy Institute, Emeryville, CA, USA; [3]Environmental Genomics and Systems Biology, Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

***Contact**: kjjardine@lbl.gov
Project Lead Principal Investigator (PI): Kolby J. Jardine
BER Program: Biological System Science Division (BSSD)
Project: This research is supported by the Office of Science Early Career Research Program (FY18 DOE National Laboratory Announcement Number: LAB 17-1761), Project: "O-acetylation and methylation engineering of plant cell walls for enhanced biofuel production (FP00007421)", Topic: Plant Systems for the Production of Biofuels and Bioproducts (Program Manager: Pablo Rabinowicz Pablo.Rabinowicz@science.doe.gov)

Project Abstract: Polysaccharides are major components of plant cell walls that can be converted into fuels by microbial fermentation, making plant biomass an important bioenergy resource. However, a substantial fraction of plant cell wall polysaccharides are chemically modified with methyl and acetyl groups that impact the yield of microbial fermentation. Although little is known about the biochemical and physiological functions of those cell wall modifications in trees, evidence suggests that they may be highly dynamic and play central roles in the control of cell growth, tissue development, and function (e.g. proper development and function of xylem vessels and leaf stomata), facilitate within and between plant signaling in response to abiotic and biotic stress, and integrate into primary C_1 and C_2 metabolism. While deesterification reactions result in the formation of volatile intermediates (methanol: meOH and acetic acid: AA) these central metabolites are not captured by traditional metabolomics analysis, representing an important gap in our knowledge of cell wall ester metabolism. Plants emit high rates of meOH, generally assumed to derive from pectin demethylation, and this increases during growth and abiotic stress. In contrast, less is known about the emission and source of AA. In this study, we connect leaf volatile emissions of meOH and AA to patterns of plant cell wall *O*-acetyl- and methyl-esters for the first time. We present a new concept of leaf cell wall *O*-acetyl/methyl ester ratios and demonstrate that they are quantitatively reflected in the AA/meOH emission ratios. *Populus trichocarpa* (California poplar) leaves in different developmental stages were desiccated and quantified for total meOH and AA emissions together with bulk cell wall acetylation and methylation content. While young leaves showed high emissions of meOH (140 μmol m^{-2}) and AA (42 μmol m^{-2}), emissions were reduced in mature (meOH: 69%, AA: 60%) and old (meOH: 83%, AA: 76%) leaves. In contrast, the ratio of AA/meOH emissions increased with leaf development (young: 35%, mature: 43%, old: 82%), mimicking the pattern of *O*-acetyl/methyl ester ratios of leaf bulk cell walls (young: 35%, mature: 38%, old: 51%), which is driven by an increase in *O*-acetyl and decrease in methyl ester content with age. The results are consistent with meOH and AA emission sources from cell wall de-esterification, with young expanding tissues producing highly methylated pectin that is progressively demethyl-esterified. We highlight the quantification of AA/meOH emission ratios as a potential tool for rapid phenotype screening of structural carbohydrate esterification patterns.

Reference

Cell wall *O*-acetyl and methyl esterification patterns of leaves reflected in atmospheric emission signatures of acetic acid and methanol (2020) Dewhirst R, Afseth C, Castanha C, MortimerJ, and Jardine K, *PLOS One* (in press).

Title: **Understanding the interplay of rooting strategy and plant hydraulic traits on the response of forest stands of CZ2 to climate variation of Southern Sierra California**

Junyan Ding[1], Polly Buotte[2], Lara Kueppers[1,2], Bradley Christoffersen[3], Mike Goulden[4], Rosie Fisher[5], Ryan Knox[1], Chonggang Xu[6], and Charlie Koven[1*]

[1]Lawrence Berkeley National Lab, Berkeley CA
[2]University of California, Berkeley, CA
[3]University of Texas, Rio Grande Valley, Brownsville, TX
[4]University of California, Irvine, CA
[5]National Center for Atmospheric Research, Boulder, CO
[6]Los Alamos National Lab, Los Alamos, NM

Contact: (cdkoven@lbl.gov)
Project Lead Principal Investigator (PI): Charlie Koven
BER Program: RGMA
Project: ECRP
Project Website: N/A
Project Abstract: Extreme droughts such as occurred in the 2012-2015 California drought are a major determinant of ecosystem disturbance and consequent impacts from and feedbacks to climate change, however these events are poorly represented in current Earth system models. Here we use a plant hydraulics model to explore ecosystem responses to the 2012-2015 California drought, in comparison with observations, for a site in the southern Sierra Nevada that experienced widespread tree mortality during the drought. We explore model parameter control of rooting depth and leaf hydraulic strategies, to identify how different plant water sourcing and photosynthetic strategies lead to different responses during normal and drought conditions. We find that deep roots are needed to match seasonal cycles of ET and GPP in normal years, an d that deep-rooted strategies also show large reductions in ET and GPP during droughts when the deep soil reservoir is depleted, in agreement with observations. We show that anisohydric leaf stomatal strategies lead to greater productivity during normal years as compared to isohydric stomatal control, but lead to high risk of xylem embolism during long-term droughts such as the 2012-2015 drought. These results show the importance of resolving plant water sourcing strategies in order to represent drought impacts and feedbacks in models.

Abiotic versus Biotic Influences on Chemical Weathering and Solute Generation in the East River Watershed

Isaac J. Larsen

[1]University of Massachusetts, Amherst, MA

Contact: (ilarsen@umass.edu)

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

BER Program: SBR

Project: Early Career project

Project Abstract: Precipitation is subject to a variety of bio-physical transformations before leaving watersheds as streamflow. One key transformation is chemical weathering, which is driven by interactions among rock, water, and biota. Globally, mountain watersheds are hotspots for solute generation, but our process-level understanding regarding the mechanisms and drivers of chemical weathering in steep, high elevation landscapes is incomplete. By employing a multi-scale approach, the project aims to address the following questions in the Rocky Mountains at the East River community watershed: 1) Does landscape-scale heterogeneity in vegetation, climate, and geology impart unique, spatially-variable signatures on soil production and chemical weathering rates? 2) What roles do the legacies of Pleistocene glaciation and Holocene geomorphic processes play in determining modern-day solute concentrations in surface waters? 3) Are physical erosion and chemical weathering rates linked at the watershed scale, and can these rates be predicted from watershed characteristics? At the soil profile scale, soil production and chemical weathering rates will be quantified with cosmogenic nuclides, specifically *in situ*-produced and meteoric ^{10}Be, and geochemical mass balance at sites that span biotic, climatic, and geologic gradients in order to isolate the key drivers of chemical weathering. At the landform scale, solute concentrations in surface waters will be used to assess whether surficial deposits generated by different geomorphic processes impart unique weathering signatures. At the watershed-scale, ^{10}Be will be used to measure erosion rates. A series of reactive transport models will be constructed to place the field-based findings into a framework for making predictions regarding the roles that vegetation, climate, and geomorphology play in solute generation.

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

Karis McFarlane[1*], Kari Finstad[1], Nina Zhang[1], Allegra Mayer[1,2]

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

Contact: (mcfarlane3@llnl.gov)

Project Lead Principal Investigator (PI): Karis McFarlane BER

Program: TES

Project: Early Career project

Project Website: na

Project Abstract:

Tropical forests account for over 50% of the global terrestrial carbon sink and 29% of global soil carbon, but the stability of carbon in these ecosystems under a changing climate is unknown.
Recent work suggests moisture may be more important than temperature in driving soil carbon storage and emissions in the tropics. However, data on belowground carbon cycling in the tropics is sparse, and the role of moisture on soil carbon dynamics is underrepresented in current land surface models limiting our ability to extrapolate from field experiments to the entire region. We measured or attained data for soil carbon stocks and radiocarbon (14C) values of profiles from over 40 sites spanning 12 pan-tropical regions. Our sites represent a large range of moisture, spanning 710 to 4200 mm of mean annual precipitation (MAP), and include Alfisols, Andisols, Inceptisols, Oxisols, and Ultisols. We found a large range in soil 14C profiles between sites, and in some locations, we also found a large spatial variation within a site. MAP explains some of the variation in soil 14C profiles and carbon stocks, with smaller C stocks and younger soil carbon in drier forests. However, differences in soil type contribute substantially to observed variation across the dataset and with constrained gradients in moisture and parent materials in Panama. We are exploring the influence of controlling factors in manipulation experiments and constrained gradients of precipitation, soil type, root inputs, geomorphology, and landuse on carbon storage and longevity through collaborative site-specific studies. For example, conversion of primary forests to pasture in the Ucayali region of Peru caused a loss of young soil carbon in 10-20-year-old pastures. Reforestation of agricultural lands restored young soil C stocks after 15 years, but these forests retain a legacy of lost carbon. Site-level runs of ELM v.1 and integration with a reduced complexity model (SoilR) are being used to evaluate model representation of soil C processes, including vertically-resolved carbon transfer rates, root inputs, and decomposition. In comparing measured soil C stocks and 14C profiles to data generated from ELMv1, we found that the model continues to overestimate carbon stock and underestimate turnover time. Finer resolution runs of ELMv1 and site-level model-data comparisons will provide more insight and be used to assess the role of climate vs other soil (e.g., soil type and parent materials) and ecosystem factors (e.g. rooting depth) in driving vertically-resolved measured and modeled soil carbon pools and ages.

Measuring and Modeling Greenhouse Gas Dynamics from Wet Tropical Forest Soils under Contrasting Redox Treatments

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

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN [2]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA [3]Department of Biosystems Engineering and Soil Science, University of Tennessee, Knoxville, TN

[4]Physical and Life Sciences Directorate, Lawrence Livermore National Laboratory, Livermore, CA

[5]Luquillo Critical Zone Observatory, Rio Grande, PR

Contact: (sihid@ornl.gov) BER Program: TES

Project: Early Career Award

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

Wet tropical forest soils frequently oscillate between fully oxygenated and anoxic conditions, which can differentially influence the dynamics of greenhouse gases such as carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O) across landscape topography. To gain a better understanding of in situ processes, we mimicked the dynamic redox oscillations in a laboratory incubation study using soil samples collected from the valley and slope topographic locations in the El Verde site, Luquillo Experimental Forest, Puerto Rico. Sixty grams of fresh soil was incubated under static oxic, static anoxic, and alternating redox conditions (every 4 days) over 76 days. The dynamics of greenhouse gases, redox-sensitive elements (total/reduced iron, ammonium, nitrite, and nitrate), extractable organic acids, pH, microbial biomass, hydrolytic enzymes, dissolved organic carbon, and organic/inorganic phosphorus were monitored on periodic destructive harvests. Overall, net CO_2, CH_4, and N_2O fluxes followed the pattern of alternating≥oxic>anoxic, anoxic>alternating>oxic, and oxic>alternating>anoxic treatments, respectively. We observed higher reduced iron concentrations and lower pH under the anoxic treatment and in the valley soils. Valley soils had greater nitrate than slope soils, especially under the oxic treatment. Landscape topography exerted an opposite effect on microbial biomass phosphorus, valley>slope, and phosphorus-degrading enzymes phosphatase and di-phosphatase, slope>valley. However, microbial biomass phosphorus and phosphorus-degrading enzymes followed a similar pattern under redox treatments (oxic>alternating>anoxic). Hence, both redox conditions and landscape topography influenced soil biogeochemistry and altered greenhouse gases dynamics. We used a geochemical modeling framework, PHREEQC, to represent the tight coupling and rapid dynamics of carbon, nitrogen, phosphorus, and iron cycles and associated greenhouse gases dynamics in wet tropical forest soils. This research will aid in understanding and predicting the high degree of variability of greenhouse gas emissions in tropical climates.

Title: Multi-Watershed Perturbation-Response Traits Derived Through Ecological Theory

James Stegen[1]

[1]Pacific Northwest National Laboratory, Richland, WA

Contact: (James.Stegen@pnnl.gov)
Project Lead Principal Investigator (PI): James Stegen
BER Program: Other
Project: Early Career
Project Abstract: *This project is focused on transforming our ability to understand and predict how the influences of biogeochemical hot spots and hot moments on surface–subsurface systems are altered by perturbation. New theory and models are being developed across a broad range of watersheds to ultimately inform next-generation Earth system models and help preserve long- term national clean water security.* A major challenge in watershed hydrobiogeochemistry is predicting how perturbation changes the influences of hot spots and hot moments over aggregate biogeochemical function. Studies of hot spot/moments are often done at single sites; these studies are powerful for revealing mechanisms, but do not immediately provide transferable knowledge and models. To enhance transferability, this study is using a multi-watershed approach that leverages existing field sites across agencies. The approach is inspired by the Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems (WHONDRS) consortium. This study also builds from the recent merging of hot spots/moments into the concept of ecosystem control points, defined as "…areas of the landscape that exert disproportionate influence on the biogeochemical behavior of the ecosystem." This notion of control points is extended here to the new concept of control point influence (CPI): the contribution of elevated biogeochemical rates in space or time to the net aggregated rate within a defined system. There are major gaps in our knowledge of how CPIs vary across systems and what drives that variation, and a need to facilitate inclusion of additional features (e.g., DOM chemistry) in state-of-the-art models. This study is revealing mechanisms underlying cross- watershed variation in CPI through a trait-based framework to predict post-disturbance CPIs across watersheds. While the trait framework can be applied to any watershed component, this project uses variably inundated hyporheic zones as a biogeochemically active, tractable model system to test underlying hypotheses and multi-watershed transferability. The trait framework couples environmental variables (e.g., stream depth variance), porewater dissolved organic matter (DOM) chemistry, and CPIs. A key element of this framework is based on an innovative application of ecological theory to highly resolved DOM chemistry analyzed via collaboration with EMSL. The focus on DOM chemistry is based on field, lab, and modeling work showing that DOM chemistry strongly influences hyporheic zone respiration rates. In addition, simulation modeling and lab experiments show strong causal associations among environmental variance, DOM chemistry, and CPIs. The hypotheses and objectives of this project are addressed by quantifying (1) spatial variation in DOM traits using broadly distributed field sampling, (2) connections among environmental traits, DOM traits, and post-disturbance CPIs using lab incubations, and (3) multi-watershed predictions of post-disturbance CPIs based on environmental and DOM traits. The study's concepts and methods can be extended to any watershed component, and outcomes can help build next-generation reactive transport models linking environmental conditions to DOM chemistry to CPI and, in turn, improved predictions of energy and material fluxes relevant to the Earth system and national water quality.

Title: Microbial Controls on Biogeochemical Cycles in Permafrost Ecosystems

Neslihan Taş[1*], Megan Dillon[1], Yaxin Xue[1], Yaoming Li[1], Craig Ulrich[1], Yuxin Wu[1], Mary- Cathrine Leewis[2], Mark Waldrop[2], Susannah Sliebner[3], Christopher Chabot[4], Rachel Mackelprang[4] and Hoi-Ying Holman[1]
[1]Lawrence Berkeley National Laboratory, [2] The United States Geological Survey, [3]GFZ German Research Centre for Geosciences Postdam, [4]California State University Northridge
Contact: ntas@lbl.gov

Project Lead Principal Investigator (PI): Neslihan Taş

BER Program: Genomic Science
Project: Early Career Research Project
Project Abstract:

The permafrost carbon reservoirs are currently protected from microbial decomposition by frozen conditions. Upon permafrost thaw microbial metabolism leads to decomposition of soil organic matter, substantially impacting the cycling of nutrients and significantly affecting the arctic landscape. **This project use state of the art molecular techniques to resolve complex microbial processes governing the biogeochemical cycles in arctic soils and permafrost to better inform efforts to access uncertainties surrounding ecosystem responses.** Permafrost microbiome is a seed bank of mostly novel organisms that have a diverse and broad metabolic potential. In-depth functional characterization of the permafrost microbes is needed to provide a foundation for understanding their responses to thaw. In order to address this gap in our knowledge we performed a pan-Arctic comparative analysis of permafrost metagenomes in which we study biogeography and metabolic functions of permafrost metagenomes assembled genomes (MAGs). This pan-Arctic analysis of permafrost MAGs across multiple locations (Alaska, Sweden, Norway, Canada and Russia) showed stark differences in microbial populations and metabolic functions that are not strong driven by environmental conditions (ice content, topography, continuity, active layer depth, and vegetation) or soil chemistry. Recognizing geospatial patterns in soil properties and microbiome characteristics across Arctic permafrost landscapes will allow us to better inform on how permafrost microbes can respond to global climate change.

The microbial response to thaw in arctic environments is not uniform and the relationship between permafrost microbiomes and greenhouse gas (GHG) emissions is not well understood. Following thaw, redistribution of water is a key event that conditions the permafrost for microbial decomposition. We initiated batch-scale permafrost incubation experiments dry, natural, and saturated moisture states and under microaerophilic or anaerobic headspaces. Via metagenomics and metatranscriptomics we dissect the microbial response leading to fermentation and competition between methanogenesis and iron and/or sulfate reduction processes, highlighting the importance of interactions between iron, sulfur and carbon metabolism. We couple omics methods with analysis of soil chemistry via synchrotron fourier transform infrared (sFTIR) spectral imaging at the Berkeley Infrared Structural Biology beamline of the Advanced Light Source (LBNL). Analysis showed that variety of organic compounds and metabolites were accumulated in thawed permafrost soils. Especially under saturated conditions while carbohydrates were depleted, soils accumulated aliphatic compounds. This project use field observations, laboratory manipulations, and multi-omics approaches to examine how microbial processes, biogeochemical transformations, and hydrology interact during permafrost thaw in different sites in Alaska in order to determine how these factors drive biogeochemical cycles.

Investigating the Impacts of Streamflow Disturbances on Water Quality using a Data-driven Framework

Charuleka Varadharajan[1*], Danielle Christianson[2], Reetik Sahu[2], Jangho Park[2], Juliane Mueller[2], Boris Faybishenko[1], Val Hendrix[2], Bhavna Arora[1], Deb Agarwal[2]

[1]Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory;
[2]Computational Sciences Area, Lawrence Berkeley National Laboratory;

Contact: (cvaradharajan@lbl.gov)
Project Lead Principal Investigator (PI): Charuleka Varadharajan
BER Program: SBR
Project: Early Career Project
Project Website: N/A
Project Abstract: Floods and droughts are projected to increase over the next few decades due to climate change. These streamflow disturbances can worsen water quality by increasing salt, nutrient, and contaminant concentrations, which will have direct consequences for human and ecosystem health. There is a pressing need to understand and predict how water quality in streams and rivers will respond to new flow- disturbance regimes. This study will determine how future changes in streamflow-disturbance events, ranging from floods to low-flow conditions, will change water quality over time. The study will use a data-driven framework consisting of data integration and analytical modules, which will be applied to the Colorado, Columbia, and Delaware River corridors.

Here we present preliminary analysis of water temperature and conductivity in the Delaware River corridor. We also describe the application of surrogate models to optimize machine-learning algorithms for prediction of daily groundwater levels in aquifers that are hydraulically connected to the Delaware River. The models use daily historical observations of temperature, precipitation, river discharge, and groundwater levels as inputs. Finally, we present tools that can be used to reproducibly synthesize diverse data for machine learning.

The outcome of this work will yield new predictions of watershed water quality characteristics, in response to extreme perturbations. The same framework will also serve as a hub to enable the generation and analysis of integrated interagency watershed datasets in real-time that are transferable to many stakeholders.

Environmental System Science

ESS-DIVE

Title: Designing the ESS-DIVE Repository to be Trusted by the Community and FAIR

Deb Agarwal[1], Charuleka Varadharajan[1], Joan Damerow[1], Shreyas Cholia[1], Val Hendrix[1], Hesham Elbashandy[1], Zarine Kakalia[1],Fianna O'Brien[1] ,Emily Robles[1], Cory Snavely[1],Karen Whitenack[1], Christopher Jones[2,3], Matthew Jones[2,3], Peter Slaughter[2,3]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2,]National Center for Ecological Analysis and Synthesis (NCEAS), Santa Barbara, CA
[3]DataONE, Santa Barbara, CA

Contact: (daagarwal@lbl.gov)
Project Lead Principle Investigator (PI): Deborah A. Agarwal
BER Program: CESD Data Management
Project: Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE)
Project Website: https://ess-dive.lbl.gov/

Project Abstract: The US Department of Energy's (DOE) Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data repository is still relatively new and growing. The focus of the repository has been on three areas of development: data access capabilities, standardization of data, and services to support projects providing data to the repository. Our approach is designed around user experience methods and involves significant discussion and involvement of the community in the design and development of capabilities. The priorities of the repository are continually revised and refined based on input from the community. We are following the developments of CoreTrustSeal and FAIR principles for data, and they are targets we hope to achieve in the future. This poster provides an overview of ESS-DIVE, its features, and the vision for the next phase of ESS-DIVE.

Title: **ESS-DIVE Publication Workflow: Publishing High Quality Data Packages with ESS-DIVE**

Val Hendrix[1], Deb Agarwal[1], Shreyas Cholia[1], Christopher Jones[2,3], Matthew Jones[2,3], Fianna O'Brien[1], Joan Damerow[1], Hesham Elbashandy[1], Zarine Kakalia[1], Emily Robles[1], Cory Snavely[4], Peter Slaughter[2,3],Charuleka Varadharajan[1], Karen Whitenack[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2,]National Center for Ecological Analysis and Synthesis (NCEAS), Santa Barbara, CA
[3]DataONE, Santa Barbara, CA
[4]National Energy Research Scientific Computing Center (NERSC), Berkeley, CA;

Project Contact: (vchendrix@lbl.gov)
Project Lead Principle Investigator (PI): Deborah A. Agarwal
BER Program: CESD Data Management
Project: Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE)
Project Website: https://ess-dive.lbl.gov/

Abstract: With the growing necessity for open access data, researchers are required to play the roles of both data provider and publisher. The Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data archive provides a publishing workflow to increase the accessibility of data produced by earth and environmental science projects funded by the Department of Energy. ESS-DIVE uses a semi-automated set of processes that result in immediate response upon publication request with subsequent easy-to-follow steps to guide data providers in preparing their data packages for publication. We will provide an overview of the ESS-DIVE publication process and describe how we use a combination of automated metadata checks coupled with a manual review checklist to efficiently publish data packages on ESS-DIVE. Using this publication workflow, ESS-DIVE moves toward meeting the challenge to efficiently disseminate diverse datasets that meet FAIR principals.

Title: Standardizing sample information to support efficient tracking, data integration, and reuse in Environmental Systems Science

Joan Damerow[1], Deb Agarwal[1], Kristin Boye[2], Eoin Brodie[1], Shreyas Cholia[1], Hesham Elbashandy[1], Kim Ely[3], Amy Goldman[4], Valerie Hendrix[1], Christopher Jones[5,6], Matthew Jones[5,6], Zarine Kakalia[1], Kenneth Kemner[7], Annie Kersting[8], Kate Maher[9], Nancy Merino[8], Fianna O'Brien[1], Zach Perzan[9], Emily Robles[1], Cory Snavely[10], Patrick Sorensen[1], James Stegen[4], Pamela Weisenhorn[7], Karen Whitenack[1], Mavrik Zavarin[8], and Charuleka Varadharajan[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA; [2]SLAC National Accelerator Laboratory, Menlo Park, CA;
[2]Brookhaven National Laboratory, Upton, NY;
[4]Pacific Northwest National Laboratory, Richland, WA;
[5,]National Center for Ecological Analysis and Synthesis (NCEAS), Santa Barbara, CA
[6]DataONE, Santa Barbara, CA
[7]Argonne National Laboratory, Lemont, IL
[8]Lawrence Livermore National Laboratory, Livermore, CA
[9]Department of Earth Systems Science, Stanford University, Palo Alto, CA
[10]National Energy Research Scientific Computing Center (NERSC), Berkeley, CA;

Contact: (JoanDamerow@lbl.gov)
Project Lead Principle Investigator (PI): Deb Agarwal, Charuleka Varadharajan
BER Program: CESD Data Management
Project: Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE)
Project Website: https://ess-dive.lbl.gov/
Project Abstract: Physical samples are foundational entities for research in earth and environmental sciences; they are not only the basis of individual studies but could also be integrated with other data to inform new and broader-scale questions. Data contributors to the Department of Energy's (DOE) Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) repository often work in large, interdisciplinary teams and send samples to multiple facilities for analyses. This community needs an efficient system for persistent sample identification to enable efficient sample tracking, data integration, and reuse.

We therefore conducted a community pilot test on the use of persistent identifiers for physical samples– specifically, International Geo Sample Numbers (IGSNs). Eight projects with a variety of sample types registered samples for IGSNs, standardized sample collection metadata, published sample metadata in the System for Earth Sample Registration (SESAR) sample catalog and have or will publish related datasets in ESS-DIVE. We compare existing sample-related standards and evaluate the experience of users to develop practical recommendations for sample identification and documentation. We gathered information for the pilot test through discussions with project teams and documented several components, such as the efficiency of the process (i.e. use of templates, labeling, registering samples, and updating metadata) and any apparent problems. We resolved uncertainties in the allocation of related sample identifiers, use of metadata elements, and added standard terms as needed. Throughout the pilot test, we also gathered feedback on desired use cases, which include: improvements in data management, advanced search capabilities, ability to link identifiers, promote interoperability of biological and geological samples, and ability to integrate and reuse sample data.

The pilot test has informed community-driven standards and tools for sample identifiers, tracking, and metadata in the ESS-DIVE repository. Our overall goal is to provide practical recommendations for efficient sample data management while also preserving and maximizing the potential value of samples into the future.

ESS-DIVE Standards: Hydrologic Monitoring and Geochemical Concentration Data and Metadata

Amy Goldman,[1*] Kristin Boye,[2*] Huiying Ren,[1] Josh Torgeson,[1] Huifen Zhou[1]

[1]Pacific Northwest National Laboratory, Richland, WA
[2]SLAC National Accelerator Laboratory, Menlo Park, CA

Contacts: (Amy.Goldman@pnnl.gov) (kboye@slac.stanford.edu) **Project Lead Principle Investigator (PI):** Deborah A. Agarwal **BER Program**: CESD Data Management
Project: Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE)
Project Website: https://ess-dive.lbl.gov/

Project Abstract: The value of archiving research data in virtual repositories in such a way that data are findable, accessible, interoperable, and reusable (FAIR) is increasingly recognized. In an effort to use the expertise of the scientific community to optimize the value of archived data within the U.S. Department of Energy's (DOE) Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) data repository, several data and metadata standardization projects were initiated as community funded projects. Here we present the standardization efforts for future data submitted to ESS-DIVE that include (1) hydrologic monitoring data and (2) water/soil/sediment concentrations of elements and/or specific chemical species.

The broad approach is similar between the two efforts: 1) review existing standards and best practices for major U.S. and global data generating projects within relevant fields, 2) discuss with DOE-ESS funded data producing scientists regarding their current best practices and willingness to adopt changes in data publication formatting, 3) examine ontologies and vocabularies for relevant parameters, 4) draft a standard and develop templates, instructions, and other documentation to support the implementation of the standard, and 5) communicate the finalized standard to the DOE-ESS community.

Our investigations have revealed broad disparity between existing vocabularies, best practices/standards, and even definitions of basic terminology (e.g., water level). Thus, there is a critical need for common agreement/acceptance among the various projects that utilize ESS-DIVE for data archiving and/or mining as to what level of constraints and requirements is acceptable/needed.

Currently we are asking for feedback on our drafted standards. We encourage all DOE-ESS community members to discuss with us so that we can ensure the standards are products that the community agrees are possible to implement and add value for both the data producers and future data users.

ESS-DIVE Standards: Leaf Physiology and Continuous Soil Respiration Data and Metadata

Alistair Rogers[1]*, Kim S. Ely[1]*, Ben Bond-Lamberty[2]*, and Stephanie Pennington[2]

[1]Brookhaven National Laboratory, Upton, NY
[2]JGCRI/Pacific Northwest National Laboratory, College Park, MD

Contacts: arogers@bnl.gov, bondlamberty@pnnl.gov
Project Lead Principle Investigator (PI): Deborah A. Agarwal
BER Program: CESD Data Management
Project: Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE)
Project Website: https://ess-dive.lbl.gov/

Project Abstract: The aim of this work is to develop standardized formats, vocabulary, and metadata requirements for both leaf-level gas exchange data and automated, continuously-measured soil respiration measurements.

The first of these efforts targets data to be uploaded to ESS-DIVE; its scope covers measurements made with portable gas exchange systems, including survey measurements of photosynthesis, respiration and stomatal conductance; response curves e.g. CO_2 response curves commonly known as A-C_i curves; and derived parameters e.g. the stomatal slope parameter. The data standard will also include specifications for other derivations of key parameters e.g. derivation of $V_{c,max}$ from proxies such as “one-point” measurements. The standard considers data output from widely used, commercially available gas exchange systems from LI-COR, PP Systems, Walz, CID Bioscience and ADC Bioscientific.

The second effort targets the nascent COSORE database (https://github.com/bpbond/cosore/), but is anticipated to provide a foundational standard for both ESS-DIVE and Ameriflux as well. This data standard covers soil respiration broadly, although COSORE targets *continuous* data in particular, and includes a careful consideration of timestamps; measured flux rates at an arbitrary number of measurement chambers at a single site, along with diagnostics associated with each flux measurement; and a variety of chamber-, instrument-, and site-specific metadata. The standard considers data output from a wide range of commercial systems, in particular the commonly-used LI-8100A, and a broad diversity of data practices.

Development of these data standards recognizes the value to the community of making raw data available, in addition to the derived parameters that form the key results of many studies. As our understanding of soil, leaf, and plant processes evolves, access to complete, raw measurement data will enable future researchers to re-process data using the new approaches; it also, we hope, will make possible future syntheses and meta-analyses powered by measurements of these globally-important carbon fluxes.

Title: **ESS-DIVE Standards for 16S Amplicon Data Products, Comma-Separated Data Files and File-level Metadata**

Terri Velliquette[1], Pamela Weisenhorn[3], Les Hook[1], Jess Welch[2], Jack McNelis[1], Ranjeet Devarakonda[1], Susan Heinz[1], Michael Crow[1].

[1]Environmental Science Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Information International Associates, Oak Ridge, TN
[3]Biosciences Division, Argonne National Laboratory, Argonne, IL

Contact: (velliquettet@ornl.gov), (pweisenhorn@anl.gov) **Project Lead Principle Investigator (PI):** Deborah A. Agarwal **BER Program**: CESD Data Management
Project: Environmental Systems Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE)
Project Website: https://ess-dive.lbl.gov/

Project Abstract: We are researching and developing generic standards for 16S amplicon abundance tables, for the data stored in comma-separated values (CSV) text format files, and for minimal file-level metadata (FLMD) schema to help data users search and locate files archived in the ESS-DIVE.

The target for the first standard is to 1) identify a typical data structure for 16S abundance tables and 2) capture the most critical provenance in machine readable format to support data re-use in models and meta- analyses, all without overburdening the original data generator. After identification of common workflows, a set of samples were run through multiple workflows with different parameterizations to examine the effects on the generated 16S amplicon abundance table to identify which factors most strongly affected the comparability of output as well as the ease of generating abundance tables in a standardized data format.
The results of this cross-workflow comparison and draft standard for 16S amplicon abundance table and provenance metadata will be presented.

This work is being done in close consultation with Systems Biology Knowledgebase (KBase) project to ensure that 16S amplicon data products stored in the ESS-DIVE repository can be seamlessly transferred to and from KBase for analysis and with the National Microbiome Data Collaborative.

To build a community supported standard for CSV and FLMD, we researched existing standards and sought feedback from ESS investigators. In this poster, we present our work thus far with preliminary thoughts on our deliverables that also include a CSV format checker and FLMD extraction scripts.

Environmental System Science

ExaSheds Pilot Project

Toward watershed simulations combining machine learning and high-resolution process-based models: Initial results from the ExaSheds project

Scott L. Painter,[1] Ethan T. Coon,[1] Dan Lu,[2] Shih-Chieh Kao,[1] Goutam Konapala,[1] Julien Loiseau[3], Irina P. Demeshko[3], J. David Moulton[4], and Carl I. Steefel[5]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[2]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, TN
[3]Computer and Computational Sciences Division, Los Alamos National Laboratory, Los Alamos, NM
[4]Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM
[5]Earth and Environmental Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: (paintersl@ornl.gov)

Project Lead Principle Investigator (PI): Carl I. Steefel (LBNL)

BER Program: Other (Data Management)

Project: ExaSheds

Project Abstract:

Sustainable management of watershed systems depends on quantitative modeling capability for the hydrologic and biogeochemical processes that control watershed system dynamics and water availability and quality. The ExaSheds project is pursuing a new watershed predictive capability that combines data-driven machine learning (ML) approaches and process-based (PB) hydrobiogeochemical simulation while taking advantage of leadership-class supercomputers. One component of that long-term vision is a PB-ML hybrid capability that uses the output of high-resolution process-based simulations as one of the inputs to ML models.

We are testing a hybrid approach using multi-decadal stream discharge data from the conterminous US-scale CAMELS dataset and short records of stream discharge from the East River, Colorado, watershed. Long Short-Term Memory (LSTM) networks were used for the ML approach and well-established semidistributed hydrology models were used for the process-based models. The hybrid approach outperforms both the LSTM and the PB approaches. For the East River catchments, the hybrid model was successfully trained using only two years of training data. These results suggest that process-based simulations can improve the robustness of ML models when inputs are out of sample and allow them to be trained with shorter records.

We used semi-distributed models as the process-based models in this initial test, but the long-term vision is to replace those with high-resolution simulations running on leadership class computers. To that end, we are also refactoring the integrated watershed simulator ATS to run on heterogeneous computing architectures that combine CPUs and GPU coprocessors. ATS was refactored using the Kokkos library, which abstracts data and execution models from the process representations, thus allowing the same code to be mapped onto a variety of computer architectures including leadership class supercomputers. Three-dimensional solutions of Richards equation on the Summit supercomputer demonstrate the feasibility of the approach.

Title: **Overview of the ExaSheds Project**

Carl Steefel[1]*, Scott Painter[2], Dave Moulton[3], Xingyuan Chen[4], Dipankar Dwivedi[1],Ethan Coon[2], Utkarsh Mital[1], J.E. Brown[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA 94720 USA
[2]Oak Ridge National Laboratory, Oak Ridge, TN
[3]Los Alamos National Laboratory, Los Alamos, NM
[4]Pacific Northwest National Laboratory, Richland, WA

Contact: (CISteefel@lbl.gov)

Project Lead Principle Investigator (PI): Steefel

BER Program: Other

Project: ExaSheds

Project Abstract:

Advances in machine learning capability, data quality and quantity, and computational capabilities create a unique opportunity to dramatically improve our watershed system modeling capability by making better use of diverse and spatially extensive data available from remote sensing, future networks of sensors, detailed site-level investigations, and highly resolved simulations. We are developing and testing a new watershed predictive capability that uses data-intensive machine learning in combination with BER's unique hydro-biogeochemical simulation capability, while leveraging leadership-class computational resources. The initial focus of the project is on the Upper Colorado River, which includes the East River Watershed under study in the Berkeley Lab SFA.

The ExaSheds seed project includes research tasks that are prototyping and evaluating strategies to address key aspects of data-driven ML applied to watershed modeling and tasks that are adapting BER's watershed computational tools to heterogeneous computer architectures. In this poster, we summarize the overall vision for the ExaSheds project and highlight some initial results. Additional results can be found in an accompanying poster led by S. Painter.

Task 1 has focused on demonstrating and evaluating the use of ML to inform watershed model inputs. For this purpose, we conducted this study at the Upper Colorado Water Resource Region (UCWRR) and used precipitation data, which is a critical forcing input for watershed models. High-resolution precipitation (<100 m) inputs are needed for accurately predicting watershed-scale hydrological and biogeochemical dynamics, but precipitation data are currently available at much coarser resolutions from PRISM (800 m; daily) and NLDAS (~12.5 km; hourly). To convert coarse-resolution precipitation data to the model resolution, referred to as "downscaling", point scale measurements are needed. To impute missing data, we used the Random Forest to learn correlations with stations that have complete records. Subsequently, we used Random Forests and Convolutional Neural Networks to generate high-resolution (~100 m) precipitation data by incorporating the effects of various factors such as elevation, vegetation, and land-use. We also identified the relative importance of these factors and examined weather station data both near to and far from the area of interest to investigate the multi-scale spatial patterns of precipitation. Results indicate that the proposed strategy generates high-resolution precipitation data by learning from lower-resolution precipitation coupled with high-resolution features with reasonable accuracy.

Environmental System Science

FACE-MDS

Title: **Help Wanted: Defining an Extensible, Understandable, and General (?) Naming Convention for Ecological and Environmental Data**

Anthony Walker[1]*, Martin G. De Kauwe[2], Paul Hanson[1], Belinda E. Medlyn[3], Richard Norby[1], Sönke Zaehle[4]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]University New South Wales, Sydney, Australia;
[3]Western Sydney University, Australia;
[4]Max Planck Institute for Biogeochemistry, Jena, Germany.

Contact: (walkerap@ornl.gov)

Project Lead Principle Investigator (PI): Anthony Walker

BER Program: TES

Project: FACE Model Data Synthesis project

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

Project Abstract: Your help is needed! Your feedback helping to define an extensible and understandable variable naming convention for ecological and environmental data would be greatly appreciated. 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. A critical element contributing to the success of the project has been a well defined protocol and QA/QC of model results. Integral to the protocol, QA/QC, and scientific analyses is the naming convention used to label the environmental and ecological data. A robust naming convention may not seem all that exciting but, agreed early in the project, the model output dataset with many variables and their associated naming convention allowed rapid assessment of model output. In many cases this assessment led to revised simulations and to the identification of bugs in the models' code. A large number of output variables also allowed in-depth assumption-centered model evaluation.

Many similar data synthesis and model inter-comparison projects exist. Thus an extensible, understandable, and possibly general naming convention would facilitate these kinds of projects. To achieve extensibility the naming convention must rely on a naming standard, that is hierarchical and ideally incorporates widely-accepted pre-existing scientific conventions. It also requires consideration of different classes of variables. We advocate for names that are readable and are broadly understandable without reference to a naming dictionary. As part of the FACE-MDS project we have been developing a naming convention with these goals in mind, but this is under development and community feedback will help to ensure many bases have been covered. At the highest level we categorise variables into mass stocks, mass fluxes, and traits (in the broadest sense). The next optional level is used for very commonly used variable names or abbreviations, e.g. GPP. The next level is to identify the location of the variable in the ecosystem, e.g leaf. Further optional levels can be used to describe finer differentiation, e.g. species. Please add your two-cents, two-dollars, or preferred currency to the conversation.

Terrestrial Ecosystem Science

University Awards

Title: **Global patterns of ecosystem legacy associated with dynamic roots and extended root turnover times in E3SM**

Max Berkelhammer[1*], Beth Drewniak[2], Miquel Gonzalez-Meler[1], Francois Ritter[1]

[1]University of Illinois at Chicago, Chicago, IL;
[2]Argonne National Laboratory, Lemont, IL;

Contact: berkelha@uic.edu

Project Lead Principal Investigator (PI): Max Berkelhammer

BER Program: TES

Project: University Project: Water foraging with dynamic roots in E3SM; The role of roots in terrestrial ecosystem memory on intermediate timescales (DE-SC0020285)

Project Abstract:

The fine root profile of ecosystems exhibits dynamic behavior in response to external forcing that influence soil moisture and the carbon pools available for root growth. However, in most Earth System Models the fine root profiles are defined by the plant functional type (PFT) and remain static in spite of external forcing. The absence of dynamic roots leads to modeled ecosystems that are unable to take advantage of available resources. However, if root profiles are too responsive to changes in soil moisture then they ultimately lose sensitivity to water and nutrient stress. This can be adjusted by modifying root turnover times such that fast turnover times increase the capacity for root profiles to respond to fleeting resource pools such as shallow water after a rain storm whereas slow turnover times lead to root profiles that have multi-year legacies. Here, we take advantage of a recently developed dynamic root module for the E3SM model to explore both how dynamic roots respond to changes in precipitation and how changes in the root profile influence the interannual legacy in ecosystems. We ran a series of 6 E3SM simulations through the historical period, which (1) either include or exclude dynamics roots, (2) have enhanced or default water sensitivity and (3) have fine root turnover times that are either default or doubled in length. Using this ensemble of simulations, we firstly compare how root profiles of the same PFT and similar mean climate state differ in response to changes in precipitation frequency (i.e. the mean interval between rainfall events). Observational data suggest that ecosystems experiencing large but infrequent rain events are going to develop deeper root profiles whereas locations with frequent small events will favor shallower roots. We will explore how this process emerges at the global scale for all PFTs and how sensitive this is to changing root turnover time. Secondly, we compare the legacy of ecosystems, defined as autocorrelation in gross primary productivity (GPP) anomalies, at seasonal to interannual timescales to assess how the combination of dynamic roots with variable turnover times influence aboveground productivity through changes in access to resources. The model results are compared against legacy assessment of the monthly SatFlux GPP product derived from OCO-2 and MODIS satellites. This work will continue through the development of a more sophisticated routine for defining root turnover times and through new observational data from a network of AmeriFlux sites.

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

Edward Brzostek[1*], Ember Morrissey[1], Zachary Freedman[1], Nanette Raczka[1], Juan Piñeiro[1], Joseph Carrara[1], Christopher Walter[1], Steve Blazewicz[2], and Peter Weber[2]

[1] West Virginia University, Morgantown, WV;
[2] Lawrence Livermore National Laboratory, Livermore, CA

Contact: erbrzostek@mail.wvu.edu

Project Lead Principle Investigator: Edward Brzostek

BER Program: TES

Project: University Award

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

To meet our objectives, we have used quantitative stable isotope probing, metabolomics, and biogeochemical approaches to quantify microbial traits and their impacts on soil C cycling across scales. Under ambient deposition, we have found that soil microbes influenced by AM trees have greater flexibility in their decomposition pathways than soil microbes influenced by ECM trees. In AM soils, the identity of the soil microbes decomposing litter as well as the resulting metabolites varied as a function of litter quality. Remarkably, in ECM soils, we found that litter quality did not result in significant shifts in decomposing microbes or metabolites. In a study of ten N fertilization experiments across the eastern United States, we have found evidence that suggests N fertilization enhances microbial C use efficiency leading to greater stabilization of C on mineral surfaces. Most recently, we have found that N fertilization reduces N use efficiency of soil microbes to the same degree in AM and ECM soils at the Fernow Experimental Forest, WV. On the modeling front, we used these results to refine our plant-microbial interactions model, FUN-CORPSE. When challenged with long-term data records from Fernow, the refined model accurately captured shifts in decomposition and the mineral stabilization of soil C in response to N fertilization. Collectively, these results highlight the importance of integrating state-of-the- art data streams into models to improve predictions of the response of temperate forests to shifts in N availability.

Title: **Sticky Roots--Implications of Widespread Viral Infection of Plants for Soil Carbon Processing in the Rhizosphere**

Zoe Cardon[1*], Marco Keiluweit[2], Carolyn Malmstrom[3], Mariela Arredondo[2], Tobias Bölscher[2], Malak Tfaily[4], Rosalie Chu[5], Rene Boiteau[6], Ellen Cole[3], Xinyu Fu[3], Kota Nakasato[3], Suzanne Thomas[1], and William Riley[7]

[1] Ecosystems Center, Marine Biological Laboratory, Woods Hole, MA
[2] University of Massachusetts, Amherst, MA
[3] Michigan State University, East Lansing, MI
[4] University of Arizona, Tuscon, AZ
[5] Environmental Molecular Sciences Laboratory, PNNL, Richland, WA
[6] Oregon State University, Corvallis, OR
[7] Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: (zcardon@mbl.edu)

Project Lead Principal Investigator (PI): Zoe Cardon

BER Program: TES

Project: University project

Project Abstract: Mineral-associated organic matter (MAOM) is a dominant component of total soil carbon that can be protected from decomposition for millennia. We are striving to understand mechanisms by which plant roots can dislodge organic matter (OM) from soil minerals. Model compounds common in rhizodeposits can destabilize MAOM, spurring its mineralization by microbes and, potentially, pulling associated nutrients into actively cycling pools. The importance of MAOM dynamics has spurred its inclusion in DOE's ELM model. We are using a novel tool to perturb belowground function: viral infection. Phloem flow is increased by infection, leading to roots becoming "sticky." Infection also decreases root:shoot ratio, so shoot nutrient demand must be met by more intensive mining of soil per unit root.

In TES Exploratory project (DE-SC0019142), we have experimented with a simple one virus (Barley Yellow Dwarf Virus)–one plant (*Avena sativa*) system. Infected plants exhibited reduced photosynthesis, plant biomass, and root:shoot ratio. Phloem contents (leaves, stems, and roots) sampled using aphid stylectomy and analyzed by GC-MS included sugars, organic acids, and amino acids. Analysis by FTICR-MS of liquid gathered from around roots of infected and uninfected plants grown hydroponically (therefore with no water or nutrient limitations) suggested a shift of rhizodeposit constituents toward amino sugars and carbohydrates with infection. Microdialysis sampling in soil microcosms, followed by LC-MS/MS, revealed altered metabolite abundances upon root growth nearby. Using synthetic MAOMs produced with ^{13}C- labeled glucose, we found that the chelator oxalic acid was most effective at mobilizing MAOM in soil slurries. In unsterilized soil, glucose and catechol were most effective, suggesting stimulation of microbial activity may have led to local conditions that mobilized MAOM.

Title: **Depth Distribution of Fine Roots and Organic Carbon Across Fertility and Rainfall Gradients in Lowland Tropical Forests of Panama**

Daniela F. Cusack[1,2*], Lee Dietterich[1], Benjamin L. Turner[2]

[1]Department of Ecosystem Science and Sustainability, Colorado State University, Campus Delivery 1476, Fort Collins, CO, 80523, USA;
[2]Smithsonian Tropical Research Institute, Apartado 0843-03092, Balboa, Ancon, Republic of Panama.

Contact: (Daniela.cusack@colostate.edu)

Project Lead Principal Investigator (PI): Daniela F. Cusack
BER Program: TES
Project: Early Career project
Project Website: https://www.facebook.com/PARCHEDpanama/?modal=admin_todo_tour
Project Abstract: Humid tropical forests contain some of the largest soil organic carbon (SOC) stocks on Earth. Much of this SOC occurs at depth in the soil profile, but the controls on SOC distribution with depth, including root inputs, climate, and soil fertility, remain poorly understood. To address this, we measured the depth distribution of SOC, fine root biomass, and nutrients in 43 lowland tropical forest soils in central Panama spanning gradients of rainfall and fertility. We hypothesized that SOC depth distributions reflect rooting depth distributions. We used fitted β parameters to characterize depth distributions, where β is a numerical index based on the asymptotic equation $Y=1–\beta^d$, in which Y is the cumulative proportion of roots or SOC to depth d. Root β values ranged from 0.82 – 0.95 across sites and were best predicted extractable potassium (K) stocks and pH. The three most acidic (pH < 4) and K-poor (< 20 g K m^{-2}) soils contained 76 ± 5 % of their fine root biomass in the upper 10 cm of the profile, while the three least acidic (pH > 6.0) and most K-rich (> 50 g K m^{-2}) soils contained only 41 ± 9 % of root biomass to that depth. Surprisingly, β values for roots were inversely related to those for SOC, such that sites with large root biomass at the surface contained large stocks of SOC in the subsoil. β values for SOC were best predicted by soil pH and base cation stocks, such that the three most base-poor soils contained 34 ± 8 % of SOC below 50 cm, while the three most base-rich soils contained only 9 ± 2 % of their SOC below this depth. Structural equation modelling suggested direct effects of K and pH on Root β, and base cations and pH on SOC β, with an endogenous relationship between Root β and SOC β. Nutrient depth distributions, in turn, were not related to either Root β or SOC β, with uniformly small stocks of nutrients at depth in infertile soils, and large subsurface nutrient stocks in fertile soils. These results suggest that global change effects on surface root growth in tropical forests are likely to have cascading effects on subsurface SOC storage, impacting large stocks of tropical C.

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

Xiao-Jun Allen Liu[1]*, Grace Pold[1], Luiz A. Domeignoz-Horta[1], Hannah Caris[1], Hannah Nicolson[1], Bhoopesh Mishra[2], Kenneth M. Kemner[3], Serita D. Frey[4], Jerry M. Melillo[5], Kristen M. DeAngelis[1]*

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

Contact: deangelis@microbio.umass.edu
Project Lead Principal Investigator (PI): Kristen M. DeAngelis
BER Program: TES
Project: University award

Project Abstract
Microorganisms mediate soil carbon (C) cycling cycling in soils as they warm over the long term, and several mechanisms mediate the warming effects on microbial physiology and climate feedbacks to the atmosphere. Microbial C use efficiency (CUE) and physical protection have emerged as major controls of microbial C processing and soil organic matter (SOM) loss and stabilization. In the Harvard Forest long-term Soil Warming Study, soils have been heated 5 °C above ambient temperature for 27 years. During this time, soils have lost almost a third of their C, which is associated with reduced substrate quantity and quality. Here we hypothesized that long-term warming reduces physical protection and CUE. We further hypothesized that long- term warming would reduce the temperature sensitivity of CUE and its components, growth and respiration. Subsamples of bulk soil at optimal moisture (~10% gravimetric) were separated into macroaggregate (250-2000 µm) and microaggregate (<250 µm) fractions. Substrate availability, microbial process rates and measures of physical protection were measured at 15 and 25 °C. Microbial CUE was determined using a substrate-independent, ^{18}O-isotope labeling method ($H_2{}^{18}O$) that quantifies the amount of ^{18}O incorporated into microbial DNA after incubation for 24 hours. We found that long-term warming reduced substrate availability (soil C and N, enzyme activity), but did not affect physical protection (*i.e.*, occluded or mineral associated SOM). Warming showed little effect on CUE, because it reduced both growth and respiration. However, CUE was reduced more at 25 °C than at 15 °C, driven by increased respiration. Long-term warming rendered CUE and its components less temperature sensitive in macroaggregates but not in microaggregates. These findings suggest that microbial thermal adaptation to climate warming occurs more among the soil fractions that are already vulnerable to degradation. We also found that physically protected C inside soil aggregates was not as degraded as inter- aggregate C (Scanning Transmission X-ray Microscopy and X-ray Raman Scattering). Analyses from the trait-based model MIMICS (Microbial-Mineral Carbon Stabilization Model) suggest that chronic warming effects on soil C were more similar to observed values when adding microbial biomass to the function of SOM physical protection. Microbial acclimation to long- term warming seems to be mediated by physical protection, potentially limiting the self- reinforcing effects of warming to the atmosphere. Our findings demonstrate the need to include physical and biochemical factors for microbial thermal strategy in Earth system models to improve predictions of soil C feedbacks to the climate system.

Climate sensitivity of peatland methane emissions mediated by seasonal hydrologic dynamics

Xue Feng[1*], M. Julian Deventer[1], Rachel Lonchar[1], G.H. Crystal Ng[1], Stephen D. Sebestyen[2], D. Tyler Roman[2], Timothy J. Griffis[1], Dylan B. Millet[1], Randall K. Kolka[2]

[1]University of Minnesota, Minneapolis, MN

[2]Northern Research Station, USDA Forest Service, Grand Rapids, MN

Contact: (feng@umn.edu)

Project Lead Principal Investigator (PI): Xue Feng

BER Program: TES

Project: University award

Project Abstract: Our project aims to guide future representations of peatland hydrology and water-carbon feedbacks within Earth System Models, by developing analytical insights and a series of parsimonious, stochastic, and process-based hydrological models that can quantify the effects of temporal hydroclimatic variability and spatial heterogeneity on peatland carbon emissions.

Recently, we used a newly developed dataset from the Marcell Experimental Forest (MEF) (Minnesota) spanning an exceptionally long 11 years to analyze the influence of soil temperature and water table elevation on peatland CH_4 emissions. We show that higher water tables dampen the springtime increases in CH_4 emissions as well as their subsequent decreases during late summer to fall. These results imply that any hydro-climatological changes in northern peatlands that shift seasonal water availability from spring to summer will increase annual CH_4 emissions, even if temperature remains unchanged. Thus, advancing hydrological understanding in peatland watersheds will be crucial for improving predictions of CH_4 emissions.

With one transect already in place, we also installed new water level loggers (in the fall of 2019) at the bog-forest boundary at MEF across three new transects to provide insight on the timing and amount of inputs to the bog from surrounding upland forests. These lateral inputs are expected to magnify the hydrological response within the bog during high intensity rainfall and snowmelt events. Currently, we are working to incorporate the seasonal dynamics of specific yield, lateral flow, and precipitation into a water balance model that will be used to predict the daily and seasonal variations in water table depths. This water balance model will be coupled to a new, stochastic reaction kinetics model to predict peatland carbon emissions in response to variable hydroclimatic forcing.

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

Sponsor Award Number: DE-SC0016188

Joshua B. Fisher[1,*], Richard P. Phillips[2,**], Edward R. Brzostek[3,**], Tom Evans[4,**], Kara Allen[3], Renato Braghiere[1], Fernando Galvan[5]

[1] UCLA, Los Angeles, CA;

[2] Indiana University, Bloomington, IN;

[3] West Virginia University, Morgantown, WV;

[4] University of Arizona, Tucson, AZ;

[5] Cornell University, Ithaca, NY

[*] PI; [**] Co-I

Contact: joshbfisher@gmail.com

Project Lead Principal Investigator (PI): Joshua B. Fisher

Project: University project

Project Abstract: Our project has advanced the science of plant-soil-microbial dynamics across these areas: i) nutrient cycling and plant uptake; ii) root exudation and priming; and, iii) mycorrhizal dynamics. Our project has accomplished 5 main developments:

1. Incorporation of phosphorus cycling into the Fixation & Uptake of Nutrients (FUN 3.0) model;
2. Coupling of FUN 3.0 into the E3SM Land Model (ELM);
3. Data collection across a large mycorrhizal gradient in the US, as well data in the tropics, to parameterize, test, and validate the model;
4. Scaling up mycorrhizal association measurements across landscapes using airborne hyperspectral remote sensing data;
5. Evaluation of global carbon and nutrient cycle impacts in the Community Land Model (CLM5.0) from a suite of new global mycorrhizal association maps.

Local and Regional Drivers of Shrub Traits in Northern Alaska

Jennifer Fraterrigo[1,2*], Weile Chen[1], Ken Tape[3], Eugénie Euskirchen[4]

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

(jmf@illinois.edu)

Lead PI: Jennifer Fraterrigo
BER Program: TES
Project: University-Led Research

Project Abstract:
Rapid warming in the Arctic is driving changes in the structure and composition of tundra ecosystems, resulting in dramatic increases in the cover of deciduous shrubs. Deciduous shrub expansion is expected to shift the distribution of aboveground and belowground plant traits, which in turn may feedback to climate by altering carbon and nutrient dynamics. However, the magnitude of this feedback is highly uncertain given limited understanding of spatial variation in plant functional traits and the over-simplification of shrub traits and their ecological effects in current ecosystem and Earth system models. To facilitate improved representation of aboveground and belowground shrub traits in models, we sampled leaf, size and root traits of common deciduous shrub species in three genera (*Betula, Alnus, and Salix*) and tussock sedge vegetation (dominantly *Eriophorum spp.*) across five moist acidic tundra sites along a latitudinal gradient in Northern Alaska (67.0 °N – 69.3 °N) and used Bayesian multilevel modeling to determine inter- and intra-specific trait relationships with local and regional environmental conditions.

We found strong interactions between site and species for most traits, indicating that interspecific trait responses covaried with regional environmental conditions. Average summer temperature and average annual climatic water deficit were the primary drivers of interspecific variation in leaf and size traits. Both shrub specific leaf area (SLA) and height increased strongly with summer temperature, while SLA, height and leaf nitrogen concentration ([N]) decreased with climatic water deficit. Root traits also covaried with climate. Specific root length (SRL) decreased with summer temperature and increased with climatic water deficit, whereas fine root density showed the opposite pattern, suggesting shrubs increase belowground carbon allocation under warmer and drier conditions. There was substantial intraspecific trait variation driven by local edaphic conditions. Shrub SLA, leaf [N], and SRL all decreased with local soil temperature and increased with thaw depth. *Eriophorum* leaf [N] also decreased with local soil temperature. These results demonstrate that there are predictable spatial environment-trait relationships at both regional and local scales that can be leveraged to model the functional consequences of climate change in tundra ecosystems.

Title: On Drought Resilience among Tree Species

Inez Fung[1*], Xiaojuan Liu[1] [1]University of California, Berkeley, CA **Contact:** (ifung@berkeley.edu)

Project Lead Principal Investigator (PI): Inez Fung

BER Program: TES

Project: High-Frequency and Vertical Variations of Soil Moisture and their Impact on Ecosystem Dynamics (DE-SC0014080)

Project Abstract:
Water is the principal regulator in biosphere-atmosphere interactions. High-frequency observations at a steep hillslope in the Mediterranean climate of northern California show that different proximate evergreen species have very different transpiration seasonality, with Pacific Madrones showing maximal daily transpiration in the dry summer season (Link et al.
2014). We hypothesize that the tree roots at the site have access to a deep store of water, as the water table some 20 meters below the surface exhibits very dynamic fluctuations with every rain storm. With DOE support, we have developed a stochastic parameterization of hydraulic conductivity that takes into account preferential flow through weathered bedrock (Vrettas and Fung, 2015), and applied the Richards Equation with the new parameterization to investigate the impact of subsurface water storage capacity (especially in the weathered bedrock) and rooting structure on the timing and magnitude of transpiration (Vrettas and Fung, 2017). The results show that it is the root mass below 4 meters that access the moisture in the weathered bedrock.
We have analyzed USDA Forestry Inventory and Analysis DataBase (FIADB) and mapped the spatial distribution of the 98 tree species in California. Our analysis shows tree mortality during the 2012-2016 drought does not map onto precipitation deficits for the period. Of the two most abundant tree species, Douglas Firs (14% of trees surveyed) experienced higher summer temperature anomalies and greater precipitation deficits than White Firs (13% of trees surveyed). Yet Douglas Firs have a mortality rate of 11% compared to 22% for White Firs. The mortality-weighted mean precipitation anomaly was -12.2 mm/month for Douglas Firs and -2.7 mm/month for White Firs, suggesting that Douglas Firs are more resilient to precipitation deficits.

We have further mapped the distribution of the tree species onto a geologic map of California. Douglas Firs are found predominantly in sedimentary rocks, while White Firs are found on plutonic rocks. Coupled with the fact that Douglas Firs have tap roots and White Firs have shallow, wide-spreading root systems, we hypothesize that sedimentary rocks, which have greater porosity than plutonic rocks, have a greater moisture storage in the subsurface, and that the moisture is accessed by the tap roots of the Douglas Firs. We thus demonstrate the interplay between climate and lithology, and show that deep water stores accessible to deep roots are not unique to the research site, and could explain differential resilience to droughts and insect infestations across a landscape.

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

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

[1]Department of Soil, Water, and Climate, University of Minnesota, Saint Paul, MN, USA;

[2]USDA Forest Service – Northern Research Station Grand Rapids, MN, USA; [3]School of Natural Resources, University of Missouri, Columbia, MO, USA; [4]University of Goettingen, Bioclimatology, Goettingen, Germany;

[5]Instituto de Investigaciones de la Amazonia Peruana, Iquitos, Peru;

[6]USDA Forest Service, Houghton, Michigan, USA;

[7]Michigan Technological University, Houghton, Michigan, USA; [8]USDA Forest Service, International Programs, Washington, D.C., USA; [9]Center for International Forest Research, Jalan, Situgede, Indonesia [10]USDA-ARS and University of Minnesota, Saint Paul, MN, USA [11]Arizona State University, Tempe, AZ, USA;

[12]Oak Ridge National Lab, TN, USA.

Contact: (timgriffis@umn.edu)

Project Lead Principal Investigator (PI): Tim Griffis **BER Program**: Terrestrial Ecosystem Sciences (TES) **Project**: University Project Award Number DE-SC0020167

Project Website: https://www.biometeorology.umn.edu/research/amazon-flux

Project Abstract:

Tropical peatlands are a major, but understudied, biophysical feedback factor on the atmospheric greenhouse effect. The largest expanses of tropical peatlands are located in lowland areas of Southeast Asia and the Amazon basin. The Loreto Region of Amazonian Peru contains ~63,000 km^2 of peatlands. However, little is known about the biogeochemistry of these peatlands, and in particular, the cycling of carbon dioxide (CO_2) and methane (CH_4), and their responses to hydrometeorological forcing. To address these knowledge gaps, we established an eddy covariance (EC) flux tower in a palm (*Mauritia flexuosa* L.f.) swamp peatland near Iquitos, Peru. Here, we report ecosystem-scale CO_2 and CH_4 flux observations for this Amazonian palm swamp peatland over a two-year period. The seasonal variation in hydrometeorology (wet versus dry seasons) had a strong effect on CO_2 and CH_4 fluxes. High air temperature and vapor pressure deficit (VPD) exerted an important limitation on photosynthesis during the dry season. Evidence from light- response analyses and flux partitioning support that photosynthetic activity was strongly downregulated during the dry seasons. The cumulative net ecosystem CO_2 exchange indicated that the peatland was a significant CO_2 sink ranging from −420 (−349 to −543) in 2018 to −455 (−384 to −542) g C m^{-2} y^{-1} in 2019. The forest was a CH_4 source of 27 (24 to 30) g C m^{-2} y^{-1}, similar in magnitude to other tropical peatlands and larger than sub-boreal peatlands. Thus, the annual carbon budget of this Amazonian palm swamp peatland appears to be a major carbon sink under current hydrometeorological conditions.

Title: **Ancient peat carbon is released as greenhouse gases following whole ecosystem warming in a northern Minnesota bog.**

Joel E. Kostka[1*], Rachel Wilson[2], Caitlin Petro[1], Tianze Song[1], Max Kolton[1], Eric Johnston[3], Christopher Schadt[3], Kostas Konstantinidis[1], Jeff Chanton[2] and Paul Hanson[3].

[1]Georgia Institute of Technology, Atlanta, GA;

[2]Florida State University, Tallahassee, FL;

[3]Oak Ridge National Laboratory, Oak Ridge, Tennessee

Contact: (joel.kostka@biology.gatech.edu)

Project Lead Principle Investigator (PI): Joel E. Kostka BER Program: TES
Project: University project

Project Website: Affiliated with SPRUCE; https://mnspruce.ornl.gov/

Project Abstract: Increases in temperature and atmospheric CO_2 concentrations have the potential to stimulate the return of stored soil C to the atmosphere as CO_2 and/or CH_4, acting as a feedback to environmental change. The Spruce and Peatland Responses Under Changing Environments (SPRUCE) project investigates the response of deep peatland C to rising temperatures and elevated atmospheric CO_2 concentrations (eCO_2) in a whole ecosystem warming experiment. This project combines advanced analytical chemistry and isotopic measurements with mult-omics approaches to elucidate the response of the belowground carbon cycle to environmental change. Early results after soil heating alone indicated that deeply buried peat was relatively insensitive to increasing belowground temperatures despite exponential increases in surface CH_4 emissions and production[1]. However, more pronounced impacts to the belowground C cycle are now observed after subsequent whole ecosystem warming[2]. Increased heterotrophic respiration was shown by accumulation of porewater CO_2 throughout the peat profile and CH_4 in the peat surface (< 50 cm). This was likely stimulated by increased availability of sugar substrates, which were shown by metabolomics to increase in concentration with warming in the surface peat. Using a combination of natural abundance stable (^{13}C) and radiocarbon (^{14}C) isotopic analysis, significant ageing of the dissolved belowground CO_2 radiocarbon signature was observed, indicating that peat plays an increasingly important role as a substrate for microbial decomposition at warmer temperatures. Specifically, evidence indicates that up to 30% of the CO_2 produced at any particular depth is directly fueled by ancient peat buried at that depth. In addition, multiple lines of evidence demonstrated that the peatland is becoming more methanogenic with warming, as shown by observed decreases in the ratios of CO_2:CH_4 and increasing ^{13}C content of CO_2 in runoff from warmed chambers. Complementary metagenomics and proteomics analyses of the microbial community are consistent with enhanced rates of methanogenesis particularly via the methylotrophic pathway. The combination of enhanced stimulation by root exudates and increasing contribution of old peat to production of CO_2 are consistent with a potential priming effect wherein highly labile substrates facilitate the decomposition of previously less bioavailable peat C compounds. The implications of this are that previously sequestered peat C appears to be mobilized with warming, contributing to a potential destabilization of the large peat carbon bank.

References:
[1]Wilson,R.M.et al.2016.Stability of peatland carbon to rising temperatures. Nature Communications 7: 13723.http://doi.org/10.1038/ncomms13723.
[2]Hopple,A.M.et al. 2020.Massive peatland carbon banks vulnerable to rising temperatures, Nature Communications,In revision

Title: **Incorporating Halophyte Hydrodynamics in Plant Hydraulics Models to Capture Mangrove Forest Responses to a Changing Climate**

Ashley M. Matheny[1*], Matteo Detto[2], Annalisa Molini[3], Chonggang Xu[4], Tim Shanahan[1], Ana Maria Restrepo Acevedo[1]

[1]University of Texas at Austin, Austin, TX
[2]Princeton University, Princeton, NJ
[3]Masdar Institute, Abu Dhabi, UAE
[4]Los Alamos National Lab, Los Alamos, NM
Contact: (ashley.matheny@jsg.utexas.edu)

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

BER Program: TES

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

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

Project Abstract: Mangroves grow along coastlines and intertidal zones, and are therefore very rarely limited by water availability. However, during the dry season, these ecosystems behave more similarly to semi-arid ecosystems than like well-watered forests. The process of salt exclusion from sea- and brackish waters during water uptake provides an additional energy and rate limiting step in the soil-plant-atmosphere continuum. Salt exclusion is responsible for high xylem tensions that result in stomatal closure and reductions in transpiration, in spite of adequate water availability. Atmospheric demand for water vapor and soil water availability are the primary determinants of vegetation water stress for terrestrial plants. Yet, in the unique case of mangroves, salinity supersedes the control of soil water availability.

We present the initial development of a salt-tolerant water uptake model for the FETCH2 advanced vegetation hydrodynamics model that will be capable of mechanistically simulating osmoregulation by halophytes. FETCH2 approximates water flow through xylem as flow through porous media and accounts for dynamic changes to conductance and capacitance of plant tissues caused by changes in water content. Parameter sets within FETCH2 are based on measurable hydraulic traits. However, studies have shown that many such traits can be highly plastic and vary spatiotemporally. Therefore, we couple our model development with an extensive field study of mangrove hydraulic traits, their variability, and their influence on plant and ecosystem level fluxes of carbon, water, and energy. Our field study analyzes mangrove forest function across both humidity and salinity gradients which are predicted to change in response to disturbances such as sea level rise, precipitation variability, inundation frequency, and increased atmospheric CO_2. We combine ecosystem scale measurements of carbon, water, and energy fluxes with plant-level observations of sap flux, biomass water content, and leaf level gas exchange in three field sites spanning a humidity gradient from Panama (humid), to the Texas Coast (subhumid), and Abu Dhabi (hyperarid). Our ultimate goal is to integrate FETCH2 into DOE's functionally assembled terrestrial simulator (FATES), to enable assessment of coastal forests in the Exascale Energy Earth System model.

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

David Medvigy,[1*] Jennifer Powers,[2] Peter Tiffin,[2] Jérôme Chave,[3] and Isabelle Maréchaux[4]

[1]University of Notre Dame, Notre Dame, IN;
[2]University of Minnesota, St. Paul, MN;
[3]CNRS, Université Paul Sabatier, Toulouse, France; and
[4]INRA, Montpellier University, Montpellier, France

Contact: dmedvigy@nd.edu

Project Lead Principle Investigator (PI): David Medvigy

BER Program: TES **Project**: University **Project Website**: n/a

Project Abstract: Liana presence can strongly suppress tree wood production and presumably also reduce the strength of the tropical forest carbon sink. In intact neotropical forests, liana presence has been increasing over the past few decades, though the mechanisms remain under debate. Better knowledge of liana morphology and allocation is required to unravel the mechanisms of below- and aboveground liana-tree competition in tropical forests and incorporate lianas into mechanistic forest dynamics models. To address these knowledge gaps, we have initiated a project that integrates empirical and modeling work.

Empirical measurements are being carried out in tropical dry forests in Guanacaste, Costa Rica, including excavations of ~80 entire trees and lianas. These excavations will enable measurements of belowground and aboveground biomass, coarse and fine root vertical distribution, and lateral root spread. Also being measured are liana soft and hydraulic traits, above- and belowground productivity, and species-level fine root productivity. The modeling work includes the incorporation of lianas into the TROLL model, which is a mechanistic, individual-based forest dynamics model. The model simulates the unique features of lianas, accounting for their structural parasitism and their different allocation strategies and morphology compared to trees. The simulated trees and lianas compete aboveground for light and belowground for water.

Thus far, 33 mature, canopy-exposed individuals (18 trees and 15 lianas) have been harvested and analyzed. For both trees and lianas, biomass partitioning to roots, stems, and leaves were consistent with the predictions of allometric biomass partitioning theory. Vertical root profiles varied across life forms: lianas had the shallowest roots, evergreen trees had the deepest roots, and deciduous trees had intermediate rooting depths. The liana root systems also had notably broader lateral extents than the tree root systems. Our empirical results have helped to motivate model development. Each of our modeled liana individuals is assigned a laterally-widespread root system that can potentially extend beneath many trees. The liana root system is then permitted to put up aboveground shoots that associate with trees within the footprint of the root system. Comparisons of simulated and observed above- and belowground productivity are currently being conducted.

Thermal Transport by Rain: A Mechanism for Warming and Thawing Frozen Soil

Joel Eklof,[1] Rebecca B. Neumann,[1*] Mark P. Waldrop,[2] Benjamin M. Jones,[3] Jing Tao,[4] Qing Zhu,[4] William J Riley[4]

[1]University of Washington, Seattle WA
[2]USGS, Menlo Park, CA
[3]University of Alaska, Fairbanks, AK
[4]Lawrenc Berkeley National Laboratory, Berkeley, CA

Contact: rbneum@uw.edu

Project Lead Principal Investigator (PI): Rebecca B. Neumann

BER Program: TES **Project**: University Project **Project Abstract**:

Northern high latitudes are projected to get warmer and wetter in the future, which will affect rates of permafrost thaw and the mechanisms by which thaw occurs. To better understand these changing thaw dynamics, we instrumented an isolated permafrost plateau in south-central Alaska with climate conditions that currently mirror those expected in more northern permafrost regions in the future. Using preliminary 2019 measurements of temperature from the soil surface into permafrost, depth to frost table, water level, groundwater temperature, and meteorological variables, we tracked soil and permafrost warming throughout the season, and identified how environmental factors, such as water table elevation, microtopography, and warm rain events, affected rates of warming and thaw. Additionally, we present the extent of permafrost degradation since the last observations at this site in 2015. These measurements indicate substantial degradation of permafrost over the past four years. Notably, collected data show rapid thaw of frozen soil within the permafrost plateau during a large rain event, providing clear evidence of the ability of rain to advect thermal energy into soils. Previous work in more northern latitudes has linked rain with soil warming within thermokarst bogs (Neumann et al. 2019) — data from this recent study identifies rain within a currently warm and wet climate as a mechanism for thawing frozen soils. This result indicates, but does not prove, that thermal transport by rain could be an important mechanisms for thawing permafrost. Capturing and correctly accounting for dynamic biosphere-atmosphere interactions and feedbacks, such as those involved with permafrost thaw, requires Earth system modeling. However, current Earth system land models, like the Energy Exascale Earth System Model Land Model (ELM), do not include transport of heat into soil from rain. Results from this and the previous study have motivated current efforts to incorporate advective heat transport within ELM, to improve its predictive capability.

References:

Neumann, R. B., Moorberg, C. J., Lundquist, J. D., Turner, J. C., Waldrop, M. P., McFarland, J. W., Euskirchen, E. S., Edgar, C. W. and Turetsky, M. R.: Warming Effects of Spring Rainfall Increase Methane Emissions From Thawing Permafrost, Geophysical Research Letters, 46, 1393–1401, doi:10.1029/2018GL081274, 2019.

Title: **Methane Fluxes from the Salt Marsh Accretion Response to Temperature eXperiment (SMARTX)**

Genevieve Noyce,[1] Teri O'Meara,[1,2] Roy Rich,[1] Peter Thornton,[2] J. Patrick Megonigal,[1]

[1]Smithsonian Environmental Research Center, Edgewater, MD;

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

Contact: (megonigalp@si.edu)

Project Lead Principle Investigator (PI): J. Patrick Megonigal

BER Program: TES

Project: University project

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

Project Abstract: The land component of the Energy Exascale Earth System Model (ELM) simulates fully coupled processes and interactions between water, energy, carbon (C) and nutrient cycles (N, P) through the ELM-PFLOTRAN interface. ELM, like most land surface models, uses soil moisture as a proxy for O_2 presence and does not track salinity, pH, or iron and sulfur cycles which are important in coastal wetlands.[1-3] Using PFLOTRAN (an open source reactive transport code), we incorporated the missing chemical interactions, plant-mediated transport of O_2, and interactions between terminal electron acceptors (e.g., aerobic and anerobic oxidation of methane (CH_4)). To test model performance, we used CH_4 emissions and porewater data collected from the Salt March Accretion Response to Temperature eXperiment (SMARTX). SMARTX was established in 2016 in the Smithsonian's Global Change Research Wetland to understand the ecosystem-scale effects of warming and elevated CO_2 on biogeochemical cycling. Year-round heating treatments range from ambient controls to 5.1 °C above ambient. Summer CH_4 fluxes from sedge-dominated areas averaged 491 µmol CH_4 m^{-2} d^{-1} in control plots, compared to 539, 571, and 1071 µmol CH_4 m^{-2} d^{-1} in plots heated to 1.7, 3.4, and 5.1 °C above ambient temperature, respectively. In grass-dominated areas, summer CH_4 fluxes also doubled with 5.1 °C of warming, from 747 to 1742 µmol CH_4 m^{-2} d^{-1}. Porewater CH_4 concentrations followed similar trends. Based on these data, we expected CH_4 emissions and dissolved CH_4 concentrations to increase exponentially with warming. However, the data from SMARTX indicate that plant-mediated transport of O_2 can mitigate warming effects, reducing CH_4 emissions. Warming effects were strongest in the grass-dominated zone, indicating effects of C substrate availability. We were able to simulate the positive influence of warming on CH_4 production while the addition of sulfate and O_2 decreased CH_4 emissions, with O_2 having the strongest influence. We found that the model was particularly sensitive to C availability. Since ELM-PFLOTRAN incorporates C processes based on terrestrial data, characterization of coastal C pool structure and decay rates are necessary to improve model simulations.

[1] Tang et al. (2016) Geoscientific Model Development 9: 927-946

[2] Thornton et al (2009) Biogeosciences 6: 2099-2120

[3] Bianchi (2007) The Biogeochemistry of Estuaries

Title: **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[6], Juan Dupuy[7], Catherine Hulshof[8], and Skip Van Bloem[9]

[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] Universidad Nacional de Colombia, Bogota, Colombia
[7] Yucatán Center for Science Investigation (CICY), Merida, Yucatán, Mexico
[8]Virginia Commonwealth University, Richmond, VA
[9]Clemson University, Clemson, SC

Contact: (powers@umn.edu)
Project Lead Principle Investigator (PI):
BER Program: TES
Project: University project
Project Website: None
Project Abstract:

Seasonally dry tropical forests (SDTFs) experience a pronounced dry season, are understudied compared to tropical rain forests, and are poorly represented in earth system models. Important knowledge gaps include: i) whether STDF are vulnerable or resistant to changing rainfall regimes, ii) how plant hydraulic traits and soil biogeochemistry vary across the dry forest biome, and iii) how nutrients and water interact to shape forest structure and function. We addressed these questions using multiple approaches including long-term observations, ecosystem-scale experiments, vegetation modeling, and surveys of plant hydraulic traits. Our results are transforming our understanding of this biome.

Long-term records of forest mortality show that a SDTF in Costa Rica is extremely sensitive to extreme drought, and that hydraulic safety margin explains interspecific variation in tree mortality. We expanded trait measurements to three other dry forests in Colombia, Mexico, and Puerto Rico that differ in rainfall regimes and soil parent material. Hydraulic traits, but not morphological traits, varied in relation to annual precipitation, rainfall seasonality and dry season length, especially when expressed as community weighted mean values. Traits conferring drought tolerance were associated with a less seasonal rainfall regime and a higher proportion of evergreen plant species, irrespective of mean annual rainfall.

We also analyzed soil samples collected during the wet and dry season from these four forests for particle size distribution, elemental composition, microbial biomass and stoichiometry, extracellular enzyme activity, net nitrogen mineralization, and phosphorus fractions. Soil biogeochemistry exhibited marked heterogeneity across the four forests: organic C, N, and P pools varied up to four-fold among sites, and inorganic nutrient pools varied over an order of magnitude. Most soil characteristics changed much more across space (i.e., among sites and plots) than over time (between dry and wet season samplings). Moreover, nutrient pools also exhibited substantial variability within forests, in some cases exhibiting as nearly much heterogeneity within a 0.25 ha plot as observed across the Neotropical dry forest biome. We observed stoichiometric decoupling among C, N, and P cycles, which may reflect their divergent biogeochemical drivers. Organic C and N pool sizes were influenced by the species composition of forest stands, particularly the relative abundance of ectomycorrhizal trees and legumes; by contrast, the distribution of soil P pools was driven by soil weathering status.

Collectively, our results highlight the functional and biogeochemical diversity of tropical dry forests, and provide datasets that can be used to improve and benchmark simulation model.

Modeling the Loading of Terrestrial Dissolved Organic Carbon to Rivers Across the Western Arctic

Michael A. Rawlins,[1*]

[1]Climate System Research Center, Department of Geosciences, University of Massachusetts, Amherst, MA

(rawlins@geo.umass.edu)

Project PI: Michael A. Rawlins BER Program: TES
Project: University Project

The quantity and quality of river discharge exported by Arctic rivers is responding to overarching influences of hydrological cycle intensification and permafrost thaw, with potential implications for the magnitude, timing, and forms of biological production occurring along Arctic coastal zones. Measurements and numerical modeling of nutrient export from Arctic rivers in recent years have supported advances in our understanding of biogeochemical cycling in Arctic coastal waters. In turn, mechanistic understanding of physical processes operating within high latitude watersheds will lead to improved predictions of the impacts of climate change on regional water and carbon exports. A permafrost hydrology model with explicit representation of soil freeze/thaw dynamics, soil organic carbon content with depth, and dissolved organic carbon (DOC) leaching in runoff was used to investigate loading of riverine DOC for the Yukon and Mackenzie Rivers, and watersheds spanning the region between them, over the period 1981- 2010. Model calibration and validation is made through multi-parameter sensitivity analysis using observational records of river discharge and riverine DOC concentrations and export.

Terrestrial DOC loading is approximately 3407 Gg C yr^{-1}, with 24.1% of the total coming from the medium and small rivers with outlets between the mouths of the Yukon and Mackenzie Rivers. The model simulations capture the observed variability in riverine DOC export dynamics and reflect the timing and magnitude of the observed DOC concentrations and stream discharge, though loading for the Mackenzie River is overestimated due to a positive bias in river discharge relative to observed annual totals. Most notably the modeling captures the characteristically high DOC concentrations observed during the spring freshet and relatively lower concentrations that arise through flow from deeper soil horizons as thaws progresses. Spatial estimates of DOC area yield and riverine DOC loading reflect the overarching influences of runoff yield, the proportion of subsurface/surface runoff, and soil organic carbon content. The model simulations point to a strong influence from DOC export on the magnitude, timing, and forms of biological production across the region's coastal zones. The synthesis of data and modeling helps to advance understanding of how climate warming manifested through water cycle intensification and permafrost degradation is likely to impact terrestrial water and carbon exports to Arctic coastal areas.

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*], Gerardo Celis[1], Justin Ledman[1], Marguerite Mauritz[1], Christina Schaedel[1], Heidi Rodenhizer[1], Meghan Taylor[1], and Yiqi Luo[1].

[1]Center for Ecosystem Science and Society, Northern Arizona University, Flagstaff, AZ

Contact: (ted.schuur@nau.edu)
Project Lead Principal Investigator (PI): Edward (Ted) Schuur
BER Program: TES
Project: University
Project Website: http://www2.nau.edu/schuurlab-p/CiPEHR.html

Project Abstract:
There are 1460-1600 billion tons of soil carbon in the northern circumpolar permafrost region, more than twice as much carbon than in the atmosphere. Understanding the magnitude, rate, and form of greenhouse gas release to the atmosphere is crucial for predicting the strength and timing of this carbon cycle feedback to a warming climate. Here we report results from an ecosystem warming manipulation where we increased air and soil temperature, and degraded the surface permafrost. We used snow fences coupled with spring snow removal to increase deep soil temperatures and thaw depth (soil warming) and open top chambers to increase growing season air temperatures (air warming). The soil warming treatment has successfully warmed soils by 2-3ºC in winter, has increased growing-season depth of ground thaw by up to 50%, and has degraded an increasing amount of surface permafrost each year of the project. 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 new measurements of ground subsidence as a metric of change in ground ice in response to permafrost thaw. To determine the impact of subsidence on permafrost thaw and soil carbon, we quantified subsidence using high-accuracy differential GPS over the course of the experiment. With permafrost temperatures already near 0°C, almost 11 cm of subsidence was observed in control plots over 9 years. Experimental air and soil warming increased the amount of subsidence five-fold and also created inundated microsites as the subsided soil surface was closer to the water table. Across treatments, the loss of ground ice was responsible for 85-91% of the subsidence, while 9-15% of the subsidence was linked to the loss of organic matter. Accounting for subsidence, permafrost thaw was 19% (control) and 49% (warming) deeper than active layer thickness measurements alone would have indicated. This corresponds to 37% (control) and 113% (warming) more carbon in the newly thawed active layer as compared to the beginning of the experiment. Ground subsidence that results in greater amounts of thawed carbon and wetter soils are not well represented by current biogeochemical models. Improved model structure that includes the physical subsidence of ground, or parameterizations that capture such effects, may be needed in order to capture the non-linear dynamics revealed by this unique long-term experiment.

Title: **Development of Artificial Roots and Synthetic Soils to Probe Mechanisms of Soil Organic Matter Cycling**

Bonnie Waring,[1*] Kenneth Smith,[1] Guopeng Liang[1]

[1]Utah State University, Logan UT

Contact: bonnie.waring@gmail.com

Project Lead Principal Investigator (PI): Bonnie Waring

BER Program: TES

Project: University Project: Leveraging synthetic root-soil systems to quantify relationships between plant traits and the formation of soil organic carbon

Project Abstract:

The balance between soil organic matter (SOM) formation and loss is regulated by dynamic interactions among plants, decomposer microorganisms, and soil minerals. However, these factors are often highly correlated in natural ecosystems, making it difficult to disentangle the mechanisms that determine the belowground fate of OM inputs. The overall goal of this project is to use artificial root-soil systems to study how C and N cycling are shaped by biotic and abiotic drivers. Data from synthetic soil incubation experiments will be used to parameterize and compare three 'microbially explicit' biogeochemical models, which make different assumptions about the dominant drivers of SOM cycling.

We present data from preliminary tests of the synthetic soils method, demonstrating that the chemical complexity of OM inputs to artificial soils regulates the size and growth efficiency of the microbial biomass. We have also developed an innovative, inexpensive, and high-throughput method to build artificial root systems that deliver customizable root exudate solutions at realistic rates in spatially discrete zones. These methods will underpin a large microcosm incubation experiment featuring a fully factorial manipulation of OM inputs, the microbial community composition, and soil mineralogical properties.

Title: **Benchmarking and developing demographic models with long-term shrub encroachment data in US tallgrass prairie**

Kevin Wilcox1, Ensheng Weng2, Kate McCulloh3, Kimberly O'Keefe3, Lydia Zeglin4, Jesse Nippert4

[1] Department of Ecosystem Science and Management, University of Wyoming, Laramie, WY, USA
[2] NASA Goddard Institute for Space Studies, New York, NY, USA
[3] Department of Botany, University of Wisconsin-Madison, WI, USA
[4] Department of Biology, Kansas State University, Manhattan, KS, USA

Contact: (kevin.wilcox@uwyo.ediu)

Project Lead Principal Investigator (PI): Jesse Nippert

BER Program: TES

Project: DE-SC0019037

Project Website: NA

Project Abstract: Shrub encroachment in the US Great Plains will likely have strong impacts on various ecosystem services, such as wildlife habitat, food production, and carbon sequestration. One overall objective of our project is to develop ecosystem demographic models to improve projections of shrub encroachment under potential future global change scenarios, and to project impacts of shrub encroachment on ecosystem services. Using simulations in a tallgrass prairie in eastern Kansas, here we show (1) developments made to an ecosystem demographic model (BiomeE) to better represent grass-shrub dynamics, (2) patterns of shrub-grass dominance and co-existence under various fire regimes, and (3) comparisons between BiomeE and FATES. Long term empirical data from the Konza Prairie Biological Station show that grass and shrub plant functional types (PFTs) co-occur in tallgrass prairie when fire occurs once every three to four years. Using BiomeE simulations, we found that growth rate differences between grass (fast) and shrub (slow) PFTs may be a primary mechanism driving three-year fire frequency necessary for coexistence. This has implications for interactions with other global change factors that alter growth rates of one or both PFTs. Additionally, a positive feedback between grass coverage and ecosystem flammability may lead to rapid ecosystem state shifts. Similarities between BiomeE and FATES demographic models are such that understanding gained from BiomeE developments should be relatively transferrable to FATES. This will provide forecasting ability for PFT shifts and their impacts on ecosystem services under various future environmental scenarios.

Title: Soil Carbon Cycling Changes at Depth Due to Woody Encroachment of Tallgrass Prairie

Lydia Zeglin[1]*, Hannah Dea[1], Rachel Keen[1], Emmett Tooley[1] and Jesse Nippert[1]

[1]Kansas State University, Manhattan, KS

Contact: (lzeglin@ksu.edu)

Project Lead Principal Investigator (PI): Jesse Nippert

BER Program: TES

Project: University project

Project Website:

Project Abstract:

The earth's land surface is covered ~40% by grass-dominated ecosystems. Shrub encroachment into grasslands is also a widespread phenomenon across the U.S. Great Plains. Woody encroachment affects ecosystem carbon (C) dynamics; however, C-cycling responses in deeper soil horizons are unknown. Understanding subsoil C responses is critical, because C stocks at depth in grassland soils are large, and encroaching shrubs have deep rooting systems. Fresh C input to subsoils could either promote C accumulation, or C loss if microbial priming of soil C mineralization occurs. We asked how shrub encroachment affects soil C cycling at depth in (a) a transitional grassland, where shrub patches exist within a grass matrix, and (b) watersheds that are shrub-invaded or remain in full grass cover. We expected higher C input and microbial activity, particularly deeper in the soil profile, under woody plants in comparison to grasses at both scales. We collected 6 replicate 1-m soil cores under dogwood islands and open grass areas at both scales, and measured soil C pools and cycling rates at 10-cm increments. Isotopic C measurements were used to differentiate C3-woody-plant-derived from C4-grass-derived pools and fluxes. Results partially support our predictions, in that the δ13C‰ of soil microbial respiration was lower under woody plants than grasses (-19.9 (1.0) < -17.1 (1.1), mean (SE), $p=10^{-16}$) over the whole soil profile, and this difference was greater at both 0-10cm and 50-100cm depths ($p=0.0002$). This shows that soil microbes use more C3-plant derived C, particularly at depth, under encroaching dogwood plants. In contrast, both total microbial respiration and the labile (30-day mineralizeable) C pool was larger and had higher δ13C‰ in grassland than woody invaded watersheds ($P<0.001$), and there was a strong positive priming response to sugar addition in grassland soils only (40-110%); but these responses did not vary significantly by depth. Total soil C had higher δ13C‰ in grassy watersheds, but total C pools had not changed even after 30 years of woody encroachment. In sum this suggests that woody encroachment of grassland changes soil C cycling, with turnover in all pools, and a net decrease in labile soil C that may be related to priming of microbial consumption of labile C. Ultimately, these data will be used in combination with linked drought experiments to better parameterize Earth System Models for forecasting the large-scale impacts of woody encroachment and drought on the grassland terrestrial C balance.

Terrestrial Ecosystem Science

Federal Agency Project

Title: **Tracking the Structural Reassembly of Puerto Rican Tropical Forests Following Hurricane Maria**

Douglas Morton[1], Ian Paynter[1,2], Maria Uriarte[3], Sebastian Martinuzzi[1,4], Veronika Leitold[5], Bruce Cook[1], Antonio Ferraz[6], Michael Keller[6,7]

[1]NASA Goddard Space Flight Center, Greenbelt, MD;
[2]Universities Space Research Association (USRA), Columbia, MD;
[3]Columbia University, New York, NY;
[4] University of Wisconsin, Madison, WI;
[5]Management and Engineering Technologies International, Inc. (METI), Washington, DC;
[6]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA;
[7]USDA-Forest Service International Institute of Tropical Forestry, San Juan, PR;

Contact: (douglas.morton@nasa.gov)

Project Lead Principal Investigator (PI): Michael Keller

BER Program: TES

Project: Multi-institutional Project

Project Abstract:

Hurricane Maria hit the island of Puerto Rico as a powerful Category 4 storm in September, 2017. Strong, sustained winds broke stems, uprooted trees, snapped branches from tree crowns, and stripped leaves from forests. Initial estimates of canopy tree damage indicated that Hurricane Maria resulted in greater damages than other recent hurricanes that hit the island, likely due to higher wind speeds and rainfall from Maria. Here, we combine pre- and post-hurricane data from forest inventory plots (2017-2020) and terrestrial laser scanning (TLS) data (2019-2020) to assess delayed mortality from hurricane damage, growth of damaged individuals, and rates of canopy closure from regrowth of canopy branches, resprouting of damaged canopy trees, and rapid growth of new individuals and understory vegetation. Field and TLS data were collected in wet forests on volcanic soils in El Yunque National Forest and moist forest on karst in Cambalache State Forest. In addition, we collected data in 2017, 2018, and 2020 using NASA Goddard's Lidar, Hyperspectral, and Thermal (G-LiHT) Airborne Imager with support from NGEE-Tropics (2017), the Department of Interior (2018), and the USDA-Forest Service (2020). High-resolution airborne data from G-LiHT provide important context for the landscape-scale heterogeneity of forest damage and recovery processes. Across the island, hurricane damages decreased fractional canopy cover by >20% , on average, and lowered average canopy height by approximately 4 m. These open conditions provided full sunlight to the forest floor, leading to rapid growth of pioneer species (e.g., *Cercropia*, *Inga*), palms (*Prestoea acuminata*), and understory vegetation, including lianas and herbaceous species. By 2020, the height of new pioneer trees reached 3-5 m, establishing a dense mid-story canopy layer comprised of both new individuals and sprouts. However, the forest canopy remained open based on the survival of damaged trees but limited regrowth of canopy branches lost during the hurricane. Together, the inventory, TLS, and G-LiHT data provide limited evidence for rapid canopy closure from canopy tree plasticity following disturbance. These findings challenge ecosystem models such as FATES to incorporate the survival and regrowth of damaged individuals and the time scales of forest recovery following catastrophic disturbance events such as hurricanes.

Terrestrial Ecosystem Science

Lawrence Berkeley National Laboratory
AmeriFlux Management Project

The AmeriFlux Management Project: Overview and the Year of Methane

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

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

(mstorn@lbl.gov)

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

AmeriFlux is a network of sites and scientists measuring ecosystem carbon, water, and energy fluxes across the Americas using eddy covariance techniques. The DOE AmeriFlux Management Project (AMP) works to enhance the value of AmeriFlux for Earth system modeling, terrestrial ecosystem ecology, remote sensing, and many other fields. In February 2020, AmeriFlux registered its 475th site, double the number of sites it had five years ago. Moreover the network has tripled the number of wetland sites and sites measuring methane fluxes. AMP is supporting operations of 14 clusters of long-term flux sites, maintaining the continuity of valuable time series of flux data. The connection with NSF's *National Ecological Observatory Network* (*NEON*) is bearing fruit, with all 47 operational NEON sites now registered in AmeriFlux and efficient data transfer between the networks. AMP has teams dedicated to four tasks: Technical support and QA/QC, Data support and QA/QC, Outreach and Network Coordination, and Core site support. Abstracts by Christianson and Pastorello describe data processing and products and by Biraud describes the Rapid Response loaner system.

AmeriFlux carried out its first theme year for network action –The Year of Methane—with a variety of events and programs. To expand and improve methane eddy covariance data, we procured and loaned three LI-COR-7700 CH_4 analyzers, offered free CH_4 calibration gases to AmeriFlux sites, and a methane sensor was integrated into AMP site visits. To enhance data usability, we added methane-related variables, like water temperature, to the Flux/Met data standard, and contributed to a FLUXNET-CH_4 data synthesis product (Knox et al. 2019). There were dedicated methane sessions at the 2018 AmeriFlux Decadal Synthesis workshop and the 2018 and 2019 AmeriFlux Meetings. The number of sites sharing CH_4 flux data increased from 13 to 34 sites.

Knox, SB, RB Jackson, B Poulter, G McNicol, E Fluet-Chouinard, Z Zhang, et al. 2019. FLUXNET-CH4 Synthesis activity: objectives, observations, and future directions. Bulletin of the American Meteorological Society, https://doi.org/10.1175/BAMS-D-18-0268.1

Scaling AmeriFlux Data Activities to Support Network Growth

Danielle S. Christianson,[1] You-Wei Cheah,[1] Housen Chu,[1] Gilberto Pastorello,[1] Fianna O'Brien,[1] Rachel Hollowgrass,[2] Yeongshnn Ong,[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, CA;
[3]University of Tuscia, Viterbo, Italy; and
[4]University of Virginia, Charlottesville, VA

(dschristianson@lbl.gov)

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

The AmeriFlux Management Project (AMP) offers diverse data services to AmeriFlux flux-tower teams and data users including: high-frequency data storage, QA/QC processing, DOIs, and standardization of flux and meteorological (flux-met) data. The network has over 475 sites, with more than 200 actively contributing data. We highlight efforts to meet increasing demand for AmeriFlux data services, primarily QA/QC of flux-met data and supporting Biological, Ancillary, Disturbance, and Metadata (BADM).

Providing standardized, QA/QC'd flux-met data to the earth science community is a core data service. The AmeriFlux BASE data-processing pipeline accepts flux-met data in a standardized half-hourly format. Automated QA/QC checks are performed and results are communicated with flux-tower teams via online reports and a customized issue tracking system. Data are then made available on the AmeriFlux website as the AmeriFlux BASE data product, which follows the FP (Flux Processing) standard. We continually add automation to the pipeline, including same-day online feedback to flux-tower teams. Data users can search over 2000 site-years (from over 270 sites) of BASE data by variable names and data years on the updated AmeriFlux Site Search webpage. BASE data is processed further, including gap-filling, flux partitioning, and uncertainty analysis, by ONEFlux, the next generation of FLUXNET processing. Evaluation data products for ~20 sites are available for download (see Pastorello et al's poster).

BADM standards (variables, units, and definitions) for non-flux data collected at sites continue to evolve. The BADM Web interface allows flux-tower teams to easily update Site General Information BADM. We released an online interface for DOI Authorship BADM to order authors and designate years of involvement. The Variable Information online tool is used by over 100 sites to provide height and instrument-model information that is shared via the Measurement Height data product. We developed a new Variable Information BADM that provides these height and instrument-model information along with variable units in the standard BADM data product format. We released the first version of these BADM with the FLUXNET2015 paper (Pastorello et al, in review).

While upgrading the 15-year-old BADM infrastructure, we tested a new submission format to collect canopy height BADM for the FLUXNET2015 paper, which has resulted in updated and expanded canopy height data for 86 AmeriFlux sites. AMP continually works to improve the flux-tower team and user experience and to increase the breadth, quantity, and quality of AmeriFlux data available for synthesis and analysis to address today's science challenges.

Integrating the ONEFlux Pipeline into AmeriFlux Data Processing Workflows

Gilberto Z. Pastorello,[1] Danielle S. Christianson,[1] Housen Chu,[1] You-Wei Cheah,[1] Abdelrahman Elbashandy,[1] Fianna O'Brien,[1] Carlo Trotta,[2] Eleonora Canfora,[2] Trevor Keenan,[1,3] Dario Papale,[2] Dennis D. Baldocchi,[3] Sebastien C. Biraud,[1] Deb A. Agarwal,[1] and Margaret S. Torn[1,3]

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

(gzpastorello@lbl.gov)

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

Gap-filled, flux partitioned data have constantly seen the highest use within the flux community. Partitioned fluxes are invaluable for running models at sites, studying physiological and ecological processes, and interpreting remote sensing retrievals. Gap-filled data are essential for analyses at different temporal resolutions and understanding long-term trends. Recognizing the significance and value of these data products, AmeriFlux is transitioning from helping to build an infrequently available FLUXNET data product to building a more regularly produced AmeriFlux product. Generation of the AmeriFlux product is being coordinated with regional networks around the globe, with initial efforts already underway, to support the continued generation of a global product. The new product builds on improvements to the current AmeriFlux BASE product, including faster QA/QC processing, further standardization of flux and meteorological (flux-met) data, and expansion of the Biological, Ancillary, Disturbance, and Metadata (BADM) templates and collection—see Christianson et al.'s poster.

By using the ONEFlux pipeline, available as an open-source collection of codes to the community, we are generating gap-filled and flux-partitioned data products for AmeriFlux sites. A collection of 20 sites is available online as an evaluation version (https://ameriflux.lbl.gov/data/download-data-oneflux-beta/), with more sites to be included throughout 2020. ONEFlux executions rely on the AmeriFlux quality control protocols, making the execution more robust and also informing new QA/QC checks to be implemented. The products in the ONEFlux pipeline include the previously mentioned (1) gap-filling of micrometeorological, flux, and other environmental variables, and (2) partitioning of CO_2 fluxes into respiration and photosynthesis, and also includes (3) the estimation of uncertainty from both the measurements and data processing steps, among other features. This poster will describe integration of the ONEFlux pipeline into AmeriFlux data workflows, highlight initial results from the evaluation sites, and discuss future development plans.

Title: The AmeriFlux Rapid Response System

Biraud C. Biraud[1], Stephen W. Chan[1], Ben Runkle[2], Rosvel Bracho[3], Ross Hinkle[4], Dave Bowling[5], Steve Kannenberg[5], and Margaret S. Torn[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]Univeristy of Arkansas, Fayettville, AR;
[3]University of Florida, Gainesville FL;
[4]University of Central Florida, Orlando, FL;
[5]University of Utah, Logan, UT

(SCBiraud@lbl.gov)

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

The AmeriFlux Management Project (AMP) technical services enable AmeriFlux to maintain high-quality data, with comparability and continuity of observations across the network, and to support innovation. The team helps AmeriFlux sites adhere to high data-collection standards and provides technical support and resources to the community.

AMP has three Rapid Response flux systems available to take advantage of unique research opportunities that come up suddenly, or may have short measurement windows. Such situations might include: measuring ecosystem fluxes following a disturbance, such as a wildfire, an infestation of borer beetles, or a habitat restoration. Site PIs may need to start measurements quickly, and/or they may plan to seek funding to purchase a new system for long-term measurements. The Rapid Response flux system can fill the gap in time or they might make measurements just for a short time.

In this poster, we will present preliminary results from three deployments of the rapid response systems:

- A plant species composition change is underway in Florida coastal wetlands, where mangrove is invading coastal wetlands. A flux tower system has been setup in a Spartina and Juncus marsh (no mangroves yet) in 2017 as part of this study. A Rapid Response system has been installed in late 2017 into a mangrove invaded Spartina Marsh (US-KS4). The pair of flux towers could provide answers to changes caused by the "lignification of graminoid marshes".
- A large-scale irrigation experiment in rice fields in Arkansas (PI: Ben Runkle, May 2019–Nov. 2020). Measuring methane emissions on adjacent fields over three growing seasons where different management practices are employed will enable researchers to quantify the degree to which this irrigation practice can reduce methane production.

A pinyon-juniper recovery following severe drought in southern Utah (PI: Dave Bowling, June 2019–May 2022). This recently installed tower at Cedar Mesa in the middle of Bear's Ears National Monument (US-CdM) will let the researchers understand how carbon and water fluxes are affected as this ecosystem recovers and/or mortality continues.

Terrestrial Ecosystem Science

Pacific Northwest National Laboratory
Soil Biogeochemistry Study

Title: **Water and Hysteretic Controls on Soil Carbon Biogeochemistry**

Kaizad Patel,[1] Jianqiu Zheng,[1] Sarah Fansler,[1] Ben Bond-Lamberty,[1,2] Vanessa Bailey[1]*

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

Contact: (vanessa.bailey@pnnl.gov)

Project Lead Principal Investigator (PI): Vanessa Bailey

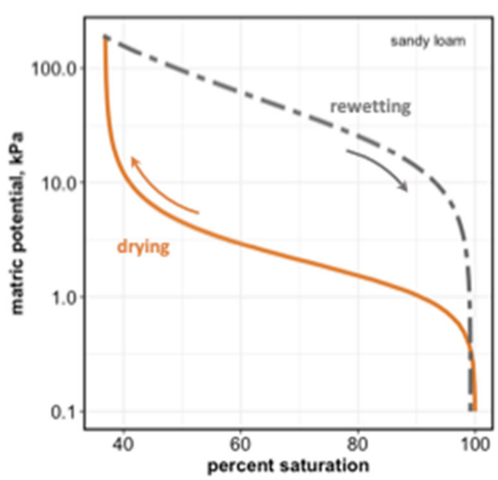
BER Program: TES

Project: PNNL TES Project

Project Abstract:

Soil organic carbon (SOC) persistence is unpredictable under extreme wetting and drying conditions, because carbon protection mechanisms are not clearly understood or well represented in models, in which the sensitivity of SOC decomposition to soil moisture is typically modeled as bell-shaped curves that relate the maximum decomposition rate to soil water content. These curves assume a linear relationship between moisture and respiration without factoring in hysteresis effects during drying and wetting that occur because different pore size domains drain in a different order than they are filled. Thus, at the same water content, the matric potential is different during draining vs. wetting events. As a result, models based on static assumptions of how soil respiration is related to soil moisture will exhibit more limited responses than real-world processes.

We are developing a process-rich understanding of how SOC physical protection under varying antecedent moisture conditions (*i.e*., drought, flood, or field-moist conditions) can improve the predictive power of models at a variety of scales. Our numerical experiments have shown a strong hysteresis effect in all simulations using empirical and mechanistic approaches. Our laboratory experiments have shown significant divergence in carbon quality and respiration rate during drying and wetting , with rewetting soils exhibiting increased levels of soil respiration and soluble SOC compared to drying soils at the same moisture level. The soluble fraction of rewet soils also had increased abundance of aromatic groups and decreased abundance of aliphatic hydrocarbons, compared to drying soils. Our results demonstrate the need to further refine the hysteresis effect on individual SOC pools in models, to accurately capture C dynamics under the influence of water.



Experiments are currently underway to investigate how (a) duration of drought influences SOC bioavailability; and (b) destabilization by pore saturation vs. increased ionic strength increases biological decomposition of SOC. We hypothesize that chemical changes due to drying are relatively static and the duration of drought will not significantly influence the chemical profile of SOC; but there will be greater differentiation with respect to the microbial community, since a longer drought duration gives the microbial community time to adapt or acclimate to the drought conditions.

Updating and applying the global soil respiration database (SRDB) for carbon cycling research

Jinshi Jian[1], Vanessa Bailey[2], Jianqiu Zheng[2], and Ben Bond-Lamberty[1*]

[1] Pacific Northwest National Laboratory, Joint Global Change Research Institute at the University of Maryland–College Park, 5825 University Research Court, Suite 3500, College Park, MD 20740, USA

[2] Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA, USA

Contact: (BondLamberty@pnnl.gov)

Project Lead Principal Investigator (PI): Vanessa Bailey, Ben Bond-Lamberty

BER Program: TES

Project: PNNL Project

Project Website:

Project Abstract:

The soil-to-atmosphere CO_2 flux (soil respiration, R_S) is the second largest carbon exchange between atmosphere and terrestrial and it plays an important role in global carbon cycling. Field R_S measurements were compiled into a global soil respiration database (SRDB) a decade ago, which has been widely used. Many new questions, however, require data which are currently not included in the SRDB. We restructured and updated the database to a new version, SRDB-V5, with several new fields collected and integrated (e.g., R_S measurement time, collar insertion depth, collar area), and older fields emended for consistency. We also updated the database from new published papers through 2017, greatly improving its spatio-temporal coverage compared with the older version.

One application of this new database involves probing the global carbon cycle for inconsistencies. For example, estimates of global GPP and R_S are typically made separately, however, and their consistency has not been previously evaluated. We show that most estimates of global GPP and R_S, typically derived from satellite-driven models and upscaled chamber fluxes respectively, are irreconcilable. Partitioning global R_S estimates into shoot and root respiration and computing the resulting GPP produces values (GPP_{Rs}, bootstrap mean 143^{+30}_{-20} Pg C yr^{-1}) significantly higher than most canonical GPP estimates (112 ± 18 Pg C yr^{-1}). Similarly, the soil respiration flux implied by GPP (Rs_{GPP}, bootstrap mean of 72 ± 11 Pg C yr^{-1}) is inconsistent (5.3%, $P < 0.001$) with canonical R_S (87 ± 9 Pg C yr^{-1}). Our findings thus demonstrate a large gap between global GPP and R_S estimates, one with implications for our understanding of global productivity, carbon turnover time, and terrestrial sensitivity to climate change.

The other application of this comprehensive global soil respiration database is to evaluate current carbon models. Currently our models vary significantly with respect to model structures, kinetic representations and the dependence and the sensitivity to key climate drivers, including soil moisture events, reflecting diverse assumptions underlying transfers of carbon among pools and representations of microbial and mineral processes. This database with extensive spatial-temporal coverage will enable systematic exploration and evaluation of current carbon models and harness the sources of uncertainties.

Terrestrial Ecosystem Science

Next Generation Ecosystem Experiments (NGEE): Arctic

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

Stan Wullschleger[1*], Robert Bolton[5], Amy Breen[5], Baptiste Dafflon[3], David Graham[1], Sue Heinz[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)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

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

Influence of Topography of Slope Terraces on the Seward Peninsula on Ground Thermal Regime, Hydrology and Development of Biogeochemical Processes

Alexander Kholodov[1]*, Amy Breen[1], Matvey Debolsky[1], and Jacob Eting[2] [1]University of Alaska Fairbanks,

Fairbanks, AK
[2]Weber State University, Ogden, UT

Contact: (alkholodov@alaska.edu)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

Slope terraces 50-200 meters width with bluffs or ridges at 2 meters high are widespread feature at the Seward Peninsula. These landforms affect the redistribution of snow during winter seasons and, thus controls soil temperature and moisture regime. It affects the vegetation and the processes of soil development. We conducted our research at one of such terraces at the milepost 28 of the Teller road. Studies included soil, vegetation and snow surveys along the 70 meters long transect, biomass productivity assessment, decomposition experiment and continuous measurements of the ground temperature and soil moisture at three points located in the rear, middle and front parts of the terrace. In according to our results mean annual ground temperature at the depth of 1.2 meters in 2019 gradually decreases from 4.2°C at the rear part to 0.5°C at the terrace's edge. Such a pattern in the ground thermal regime is mostly caused by the difference in winter temperature due to snow redistribution. The soil moisture regime might be identified as ***Ustic*** at the rear and middle parts and ***Udic*** at the front of the terrace. Across the tread of the terrace vegetation changes from the grassland in the rear part to ericaceous tundra in the middle and lichen tundra at the front. Aboveground productivity increases from rear (449.6 g/m^2) to front part (1099.76 g/m^2) of the terrace. But it is necessary to notice that 87% of production in the frontal part represented by lichens. Significant portion (66.8%) of the total biomass of the ericaceous tundra composed by woody species, so only about a one third (816.6 g/m^2) of it can be involved in the process of annual carbon turnover as a litter. Rear part is only a section of the terrace where the whole annual harvest of biomass turns in a litter. Thus, an amount of annual litter biomass decreases from the rear to frontal pert. The highest rate of litter decomposition was recorded at the middle section of terrace and the lowest – at the front. Processes of the organic stabilization was the lowest at the rear part of the terrace. Combination of all about mentioned factors and processes explain the pattern in soil sequence. The most developed soil profile (***Ustic Haplocryols***) can be found at the rear part of the terrace replacing by the ***Typic Humicryepts*** at the middle and ***Typic Dystrogelepts/Haplogelepts*** at the front.

Quantifying the Influence of Bedrock, Soil, Snowpack, Topography and Vegetation Properties on Subsurface Thermal Regimes across an Arctic Watershed in a Discontinuous Permafrost Environment

Baptiste Dafflon[1]*, Sebastian Uhlemann[1], Ian Shirley[1], Patrick McClure[1], Stijn Wielandt[1], Carlotta Brunetti[1], John Peterson[1], Craig Ulrich[1], and Susan Hubbard[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA Contact: (bdafflon@lbl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

In Arctic regions, quantifying the soil and bedrock properties, their thermal-hydrological behavior and their links with landscape properties is particularly challenging yet critical for predicting the storage and flux of carbon and water in a changing climate. This study aims at improving the quantification of subsurface properties and thermo-hydrological fluxes, and their interactions with ground surface and vegetation properties in discontinuous permafrost environments. Our work takes place in a watershed along Teller road near Nome (Alaska) and is part of the Next-Generation Ecosystem Experiments (NGEE-Arctic). The watershed shows significant heterogeneity in vegetation, snowpack, geomorphic and subsurface characteristics.
We use a variety of aerial and ground-based measurements, including electrical imaging, seismic refraction, geophysical well logging, a Distributed Temperature Profiling (DTP) system, CO_2 efflux and water content measurements, soil sample analysis, and UAV-based mapping of snow thickness and vegetation characteristics. Data analysis is performed following an ecosystem-type construct to identify how areas with distinct distribution of above- and belowground properties can be delineated using remote sensing products and a limited amount of ground-based measurements. The data analysis is supported by numerical approaches that simulate hydrological, thermal and biogeochemical processes. Overall, this study enables the identification of watershed structure and associated subsurface and landscape properties. Our unique dataset has highlighted significant relationships between above- and belowground characteristics including: (1) the effects of topographic lows and tall shrubs on thick snowpack and talik distribution; (2) the significant spatial co-variability between permafrost characteristics, soil properties, vegetation, and geomorphology, with graminoid covered areas corresponding to zones having the shallowest permafrost table; (3) the rapid soil thermal-hydrological responses to snowmelt and intense rainfall events, and the increasing permafrost thaw following thick snowpack year, as imaged by automated monitoring of electrical resistivity, temperature and moisture; and (4) the significant influence of soil hydrological and thermal behavior on soil CO_2 efflux. Further, numerical models with adequate parameterization and level of process representation improve our understanding of how near-surface permafrost transitions to talik and absence of permafrost. The obtained information is expected to be useful for improving predictions of Arctic ecosystem feedbacks to climate.

Simulating Iron Reduction and Methanogenesis in Arctic Soils Using PFLOTRAN and ELM

Benjamin Sulman[1], Fengming Yuan[1], Teri O'Meara[1,2], Elizabeth Herndon[3], David Graham[4], Baohua Gu[3], and Peter Thornton[1]

[1]Climate Change Science Institute and Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Smithsonian Environmental Research Center, Edgewater, MD
[3]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[4]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: (sulmanbn@ornl.gov)
Project Lead Principle Investigator: Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

Biogeochemical cycles in thawing permafrost soils depend on interactions between carbon, nitrogen, microbial decomposers, and terminal electron acceptors. Redox cycling of iron (Fe) plays an important role in thawing permafrost soils. Reduction of Fe(III) to Fe(II) provides a preferential pathway to organic matter mineralization over methanogenesis, potentially decreasing methane production rates while Fe(III) is available. Fe(III) availability is dependent on soil minerals and pH as well as total dissolved Fe concentrations. Oxidation of Fe(II) at the oxic/anoxic interface and during cycles of inundation and oxygen exposure can play an important role in Fe(III) availability by replenishing reducible Fe. Land surface models such as the E3SM Land Model (ELM) currently do not simulate dynamics of either terminal electron acceptors or pH, instead assuming that water table and time since inundation can be used as proxies for controls on anaerobic decomposition pathways. We simulated organic matter degradation, Fe(III) reduction and Fe(II) oxidation, and methanogenesis in the reactive transport model PFLOTRAN and used an established interface to couple it to ELM. Model simulations were compared with measurements of Fe cycling and methane production from laboratory incubations. Simulations of inundation/oxygenation cycles showed that Fe availability and mineral properties drove the temporal dynamics of methanogenesis, with the onset of maximum methane production controlled by the rate of Fe(III) depletion. Incorporation of redox processes into ELM via PFLOTRAN will improve model simulations of CO_2 and CH_4 emissions from soil systems with dynamic hydrology and biogeochemistry, which are particularly important in the Arctic.

21st Century Tundra Shrubification Controlled by Non-Growing Season Plant Nutrient Uptake

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

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

Contact: (wjriley@lbl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

The role of plant photosynthesis in controlling high-latitude tundra carbon stocks is strongly limited by nutrient availability and critical for centennial-scale climate interactions. However, global land model plant representations are uncertain and fared poorly in recent confrontations with high-latitude observations. We show here that tundra plant nutrient acquisition during the non-growing season (NGS), a widely observed process ignored by most large-scale land models, is substantial and affects modeled ecosystem vegetation composition and carbon budgets. We apply a well-tested mechanistic model of coupled plant, microbial, hydrological, and thermal dynamics that explicitly represents nutrient acquisition based on competitor traits. We further test the model against observed NGS plant nutrient uptake in a northern Alaskan tundra site and then demonstrate strong effects of NGS nutrient uptake on plant growth. Applying the model across the North America tundra indicates that NGS nutrient uptake is consistent with observations and ranges between ~5-50% of annual uptake, with large spatial variability and dependence on plant functional type. Finally, we show that NGS plant nutrient acquisition strongly enhances 21st century tundra shrubification rates. Our results highlight the importance of NGS plant and soil processes on high-latitude biogeochemistry and vegetation dynamics and motivates new observations and processes to represent these dynamics.

Factors Influencing Soil Moisture at Field Sites on the Seward Peninsula, Alaska

Julian Dann[1], Robert Bolton[2*], Lauren Charsley-Groffman[1], Richard Chen[4], Elchin Jafarov[1], Emma Lathrop[1], Mahta Moghaddam[4], Dea Musa[1], Stan Wullschleger[3], and Cathy J. Wilson[1*]

[1]Los Alamos National Laboratory, Los Alamos, NM [2]University of Alaska Fairbanks, Fairbanks, AK [3]Oak Ridge National Laboratory, Oak Ridge, TN [4]University of Southern California, Los Angeles, CA

Contact: (cjw@lanl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

Soil moisture plays a key role in Arctic ecosystems because it is a control on the carbon cycle, vegetation, and energy balance. Researchers in the DOE Office of Science Next-Generation Ecosystem Experiments (NGEE-Arctic) and the NASA Arctic Boreal Vulnerability Experiment (ABoVE) projects are collaborating on the development of regional soil moisture data products to improve and assess Earth System Model predictions. Here we present analysis of in-situ measurements of soil moisture and thaw depth collected during the Summer of 2017 coincident with NASA ABoVE airborne overflights of a P-band synthetic aperture radar (SAR) instrument called AirMOSS. At each in-situ soil moisture location, consistent measurement techniques were used including the establishment of multiple 100m by 100m plots designated for ground-truthing in accordance with ABoVE protocols to ensure a representative measure of soil moisture based on the resolution of the SAR instrument. Remotely sensed soil moisture is derived from the SAR imagery using a two-layer dielectric model within the active layer (Chen et al. 2018). Using a non-linear generalized additive model (GAM) we quantify the impact of topography, geomorphology, and vegetation on the SAR-derived soil moisture product across a large swath of the Seward Peninsula. These observations and analyses provide a unique benchmark dataset with which to test predictions of spatial variation and temporal evolution of soil moisture in local and regional permafrost models. Results of this study suggest that soil moisture on the Seward Peninsula is driven primarily by slope, vegetation type, and aspect.

High-Resolution Mapping of Ice Wedge Polygons for Environmental Applications

Charles Abolt[1*], Michael Young[2], Adam Atchley[1], Dylan Harp[1], Vitaly Zlotnik[3] and Cathy Wilson[1]

[1]Los Alamos National Laboratory, Los Alamos, NM [2]The University of Texas at Austin, Austin, TX
[3]University of Nebraska-Lincoln, Lincoln, NE

Contact: (cabolt@lanl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

It is well known that microtopography associated with ice wedge polygons drives pronounced, meter-scale spatial gradients in hydrologic and ecological processes on the tundra. However, high-resolution maps of polygonal geomorphology are rare, due to the complexity and subtlety of ice wedge polygon relief at landscape scales. Here we present a novel method to rapidly delineate and measure the microtopography associated with individual ice wedge polygons within high-resolution digital elevation models (DEMs). At its core, the method relies on a convolutional neural network paired with a set of common image processing operations to segment a DEM into discrete polygons. The relief at the center relative to the periphery of each polygon is then calculated, placing each instance on a spectrum between low-centered and high- centered endmembers. The robustness of the method is demonstrated through application across a ~1,200 km^2 landscape south of Prudhoe Bay, capturing $>10^6$ individual polygons. Manual validations suggest that the results at both spatial scales are highly accurate; in general, >90% of polygons extracted by the algorithm are correctly delineated. The resulting maps permit visualization of heterogeneity in ice wedge polygon geomorphology with unprecedented detail, revealing complex patterns in the spatial distribution of low-centered and high-centered polygons across diverse landforms. We demonstrate one application of the map, by using it to parameterize a simple analytical model of groundwater flushing from the active layer of ice wedge polygons. The results place an upper bound on the landscape-scale flux of water from polygonal soils into thermokarst troughs, which may represent an important pathway for mobilization of dissolved organic carbon and other nutrients.

Biogeochemical Redox Interactions Modulate Soil Organic Matter Mineralization in Wet Arctic Tundra

David Graham[1*], Michael Philben[2,3], Lijie Zhang[2], Neslihan Taş[4], Adam Klibisz[1], Jianqiu Zheng[1,5], Baohua Gu[2], and Stan Wullschleger[2]

[1]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN [2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN [3]Geological & Environmental Science, Hope College, Holland, MI [4]Earth & Environmental Sciences, Lawrence Berkeley Laboratory, Berkeley, CA
[5]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA

Contact: (grahamde@ornl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov

Wet Arctic tundra stores organic matter under conditions that limit oxidation, protecting soil C from mineralization. Prediction of greenhouse gas emissions from these sites will require modeling interactions among biotic and abiotic redox processes. The NGEE Arctic study site northwest of Nome, Alaska includes a small watershed with varying terrain and plant types. Near the top, a degraded peat plateau is underlain by mineral- and ice-rich permafrost. At the toe of the hillslope, tussock tundra intermixes with standing water and sedge-rich pools over degraded permafrost. Soil O horizons in both areas contain substantial stocks of soil organic matter.
Mineral soils generally have a sandy clay loam texture, and soil water content correlates with soil C and N as well as P, S and K. Diverse microbial communities catalyze a cascade of decomposition and redox reactions in the soils. Anoxic incubations of toe slope soils produced more CO_2 and CH_4 than plateau soils, fueled by higher concentrations of water-extractable organic C and mineral composition. These incubations showed rapid reduction of sulfate and Fe(III), followed by increased methanogenesis. Addition of molybdate inhibited the already low rate of sulfate reduction in the toe slope soil. Microbial community analysis identified members of two major types of methanogens: the acetoclastic family Methanosaetaceae and the hydrogenotrophic Rice Cluster II. Methanogen activity was inhibited by bromoethanesulfonate. Summer field campaigns measured redox-active species in soil pore waters. CH_4 and CO_2 concentrations were low in pore waters from the peat plateau and higher in the toe slope, consistent with incubation results and nutrient transport. Methane increased with depth and pH, while dissolved organic carbon and phosphate decreased with depth. CH_4, CO_2, and Fe(II) concentrations were correlated in pore waters, indicating contiguous anaerobic respiration processes. Concentrations of oxidized anions NO_3^- and SO_4^{2-} correlated with dissolved organic carbon and organic acids. These were more abundant in toe slope soils possibly due to nutrient transport from the hillslope. Although most soil water samples were undersaturated in dissolved oxygen, even deep pore waters that contained substantial amounts of dissolved Fe(II) had more than 2 mg/L dissolved oxygen. These results characterize the wet tundra of the Teller Road site as suboxic, where a complex mix of dissolved O_2 and redox-active ions can interact and influence soil organic matter decomposition and greenhouse gas emissions.

MODEX Approach to Diagnose and Improve Snow Processes and Phenology in E3SM Land Model (ELM) in Northern High-Latitude Regions

Fengming Yuan*[1], Daniel Ricciuto[1], Min Xu[1], Nathaniel Collier[1], Xiaoying Shi[1], Dali Wang[1], Forrest Hoffman[1], Peter Thornton*[1], and Stan Wullschleger[1]

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

Contacts: yuanf@ornl.gov, thorntonpe@ornl.gov
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov

In high-latitude Arctic, modeling land surface processes, e.g. snow, relevant phenology, and consequent soil and plant responses are of great challenge in Earth System, mostly due to highly heterogeneous surface across scales and lacking reliable data in those remote and harsh regions. In this study, we present an offline land surface simulation using Energy Exascale Earth System Model's (E3SM) Land Model (ELM) over northern high-latitude regions (>=60ºN) at half- degree spatial resolution. This offline ELM is driven by GSWP3 (Global Soil Wetness Project Phase 3) v2 forcing data from 1901-2015. Model results are evaluated using ILAMB tool package and NCAR Land Diagnosis Tools (as shown on https://elm-ngee-webserver.ornl.gov). Improvement aiming to high resolution pan-Arctic modeling via model development and experiment data integration (MODEX) are explored in NGEE Arctic Project. By using ILAMB tools and available datasets, we find that ELM simulation of vegetation LAI and total soil organic matter (SOM) remarkably well, but still mismatch both spatially and temporarily.
Severe under-estimation of LAI (and thus SOM) and phenological shifts apparently exists in Northeastern Siberian Russia and Northeastern Canada. Regional analysis by NCAR Land Diagnosis Tools reveals that such bias can be tracked back to both snow-fall data in model forcing, e.g. heavy or extended winter snowing, and model snow processes and consequent phenology. Station-level snowfall and snow depth observations at VanKarem, Northeastern Siberian Russia, for an example, demonstrated that snowfall in GSWPv2 forcing data could be too high, which caused ELM snow melt lasting until mid-July and thus short growing seasons especially for heavy-snowing winters. At another exampled station at Alert, Canada, historical air temperature and snowfall are comparable to GSWPv2 forcing, but ELM simulated much deep snow and very short snow-free period compared to the observed. Initial tests show that snowfall adjustments and ELM snow or phenology modification can improve model performance in relevant regions. It implies that both data integration and model development and assessments are critical to further improve ELM performance in pan-Arctic.

Patterns and Drivers of Alder Distribution Across a Tundra Landscape at Seward Peninsula

Forrest M. Hoffman[1*], Jitendra Kumar[2], Venkata Shashank Konduri[1], Verity G. Salmon[2], and Colleen M. Iversen[2]

[1]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: (forrest@climatemodeling.org)
Project Lead Principal Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov

Arctic regions have exhibited a greening trend and rapid expansion of deciduous shrubs across previously graminoid-dominated tundra vegetation communities. Among tundra shrub species, Alders (*Alnus*) are of key interest due to their ability to fix biologically available nitrogen to the ecosystem via symbiotic nitrogen fixation. *Frankia alni* bacteria living within Alder root nodules fix nitrogen in exchange for plant-produced carbohydrates. As an early successional species, Alders often colonize disturbed areas with low levels of nitrogen availability such as river and stream floodplains, fire burned areas, and cryoturbated mineral soils. Their significant contribution to high latitude greening highlights the need for understanding their current distribution across tundra landscapes and environmental conditions supporting their expansion and establishment. Using a machine learning-based approach we are analyzing high resolution satellite remote sensing data set to understand the current distribution of Alder shrubs across the Seward Peninsula of Alaska, where the US Department of Energy's Next Generation Ecosystem Experiments (NGEE) Arctic project is conducting field, laboratory and modeling-based studies. Using field observations collected during the 2017–2019 field seasons, we are training deep learning models to classify the current distribution of Alder shrubs across the topographically complex landscape. By analyzing the topographic, hydrological, edaphic and micro-climatic conditions in the regions of known Alder presence, we are investigating the patterns of Alder expansion and establishment. As the vast Arctic tundra landscape experiences a warming climate, understanding the drivers of Alder expansion and establishment will inform predictions of potential regions where shrubification may occur. With its ability to fix nitrogen, Alders also modulate the nutrient cycle and vegetation communities in the broader landscape. Our research will also shed light on the biogeochemical impacts of Alders on tundra ecosystems.

Mapping Arctic Vegetation using Hyperspectral Airborne Remote Sensing Data

Shashank Konduri[1], Jitendra Kumar[2], Forrest Hoffman[1*], and William Hargrove[3]

[1]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, TN
[2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN
[3]US Forest Service, Southern Research Station, Asheville, NC

Contact: (konduriv@ornl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov

Amplified warming in the circumpolar Arctic has led to shifts in vegetation composition, increased shrubification and northward expansion of tree line. Changes in Arctic vegetation cover and composition are likely to have a significant impact on tundra ecosystem function through changes in hydrological regimes, energy exchange, and carbon and nitrogen cycling. Understanding the current composition and distribution of vegetation is essential for studying this sensitive ecosystem and predicting responses to environmental change. Mapping Arctic vegetation from coarse spectral- and spatial-resolution satellite remote sensing data is challenging because of poor image quality due to persistent cloud cover and polar darkness, in addition to the high diversity and heterogeneity of vegetation. Our analysis is focused on the Seward Peninsula of Alaska, where the US Department of Energy's Next Generation Ecosystem Experiments for the Arctic (NGEE Arctic) project is conducting in situ measurements. Using airborne hyperspectral remote sensing data from NASA AVIRIS-NG and satellite remote sensing platforms, we are developing high resolution maps of vegetation community distribution and estimates of fractional plant functional type (PFT) distributions for models. We are developing and applying deep learning models, trained using field-based vegetation community survey observations, for remote sensing-based classification of vegetation communities. High resolution maps of vegetation for Seward Peninsula will be used to understand environmental controls on patterns of vegetation distribution on the landscape, while estimates of PFT distributions will inform and improve the representation of vegetation dynamics in Earth system models.

The Effects of Talik Formation on Non-Growing Season Carbon and Nitrogen Cycling Permafrost Ecosystems

Ian Shirley[1,2*], Baptiste Dafflon[2], Haruko Wainwright[1,2], Zelalem Mekonnen[2], Bhavna Arora[2], William Riley[2], and Susan Hubbard[1,2]

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

Contact: IShirley@lbl.gov
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

High-latitude warming is expected to increase talik formation -- a unit of unfrozen body in subsurface -- in permafrost across the arctic. The appearance of a perennially unfrozen soil layer represents a drastic shift in subsurface hydrology and is expected to have a significant impact on carbon and nitrogen cycling, especially during the winter months. In this study, we use an integrated ecosystem model, *ecosys*, to investigate how the presence or absence of a talik shifts the connectivity and dependency of key hydrological controls on non-growing season carbon and nitrogen cycling in permafrost ecosystems. Our work focuses on a watershed along the Teller road on the Seward Peninsula in Alaska that has been extensively characterized and monitored by the Next-Generation Ecosystem Experiment (NGEE Arctic). First, we apply a Morris global sensitivity analysis to explore how the observed variation in topography, soil properties, and meteorological inputs across the watershed affects modeled soil temperatures. We then split the model runs into two groups based on the presence or absence of a talik within the run and apply a Bayesian network approach to interpret the complex and interrelated model outputs. Separate Bayesian networks are developed based on the two groups of runs using a constraint-based hill- climbing algorithm. Differences in the network structure are used to interpret how the relationships between key variables for wintertime soil carbon and nitrogen transformations and the exports changes under the talik formation.

A Mechanistic Model of Climate Sensitivity Hysteresis of Soil Organic Matter Dynamics

Jinyun Tang[1*] and William J. Riley[1]

[1]Earth & Environmental Science Area, Lawrence Berkeley National Laboratory, Berkeley, CA Contact:

(jinyuntang@lbl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov

Empirical observations have indicated that the climate sensitivities—temperature and moisture— of soil organic matter (SOM) decomposition are very likely hysteretic. However, most existing models of SOM dynamics assume these climate sensitivities as deterministic, leading to predictions that are lacking observed temporal variability, and degrading the credibility of projected long-term SOM dynamics. We here use first-principle-based theories to assemble a SOM model that explicitly resolves the interactions between microbes, substrates, enzymes, mineral surfaces, and physical transports. The model makes predictions of hysteretic responses of SOM decomposition to changing temperature and moisture conditions that are consistent with a range of empirical observations. Since our model also predicts important emergent parameters (e.g., carbon use efficiency, substrate affinity, etc.) that are treated as constant in other models, it allows us to demonstrate that it is the lack of parametric variability that makes the traditional response function-based models to underestimate the climate sensitivities of SOM dynamics, and overestimate the predictive uncertainty resulting from the parametric equifinality. We further discussed how our approach can be extended to improve the modeling of other climate sensitive soil biogeochemical processes.

Quantifying the Controls of Permafrost-Dominated Hillslope Processes on both Gradual and Catastrophic Soil Movement

Rachel Glade[1], Michael Fratkin[1], Joanmarie DelVecchio[2], Mara Nutt[1], and Joel Rowland[1*] [1]Earth &

Environmental Science Division, Los Alamos National Laboratory, Los Alamos, NM
[2]Department of Geosciences, Pennsylvania State University, University Park, PA

Contact: (jrowland@lanl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

Arctic soil movement, accumulation and stability exert a first order control on the fate of permafrost carbon in the shallow subsurface and landscape response to climate change. A major component of periglacial soil motion is solifluction, in which soil moves as a result of frost heave and flow-like "gelifluction". Because solifluction soil is a complex granular-fluid-ice mixture, its rheology and other material properties are largely unknown. However, solifluction commonly produces distinctive spatial patterns of terraces and lobes that have yet to be explained but may help constrain solifluction processes. Here we take a closer look at these patterns to better understand material and climatic controls on solifluction. We find that the patterns are analogous to classic instabilities found at the interface between fluids and air—for example, paint dripping down a wall or icing flowing down a cake. Inspired by classic fluid mechanics theory, we hypothesize that solifluction patterns develop due to competition between gravitational and cohesive forces, where grain-scale soil cohesion and vegetation result in a bulk effective surface tension of the soil. We show that, to first order, calculations of lobe wavelengths based on these assumptions accurately predict solifluction wavelengths in the field. We also present high-resolution DEM-derived data of solifluction wavelengths and morphology from dozens of highly patterned hillslopes in Norway to explore similarities and differences between solifluction lobes and their simpler fluid counterparts. Ongoing studies on the Seward Peninsula along the Teller Road seek to understand how gradual slow movement, such as solifluction, have led to the development of hillslopes, burial of soil organic carbon, and control the sensitivity of hillslopes to rapid failure. At the Teller 47 field site, numerous active layer detachments occurred in 2019 following an extreme summer precipitation event. This site has also experienced significant hillslope and failures and gullying prior to 2019. Through field and drone-based mapping of failures, combined with subsurface investigations we seek to understand why the hillslope at Teller 47 appear particularly sensitive to thaw-related failures and erosion.

Understanding Snow Patterns for Improved Earth System Modeling in the Arctic

Katrina Bennett[1*], Julian Dann[1], Emma Lathrop[1], Robert Busey[2], William Bolton[2], Baptiste Dafflon[3], and Cathy Wilson[1]

[1]Los Alamos National Laboratory, Los Alamos, NM [2]University of Alaska Fairbanks, Fairbanks, AK
[3]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: (kbennett@lanl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

In the Arctic, changes to snow patterns are resulting in shifts to eco- and hydro- system functioning. In this region of the world, shifts in snow properties have reverberating effects on permafrost, ecology, and biology, with notable feedbacks between atmospheric moisture, sea ice, and albedo. While in the lower latitudes, shifts in high elevation snow is largely owing to changes in temperature, the Arctic cryosphere exhibits strong coupling between changes in snow, atmospheric moisture transport, and soil and air temperatures. The Next Generation Ecosystem Experiment (NGEE)-Arctic has been working to understand how changing snow patterns affect evolving permafrost and vegetation on the Seward Peninsula, Alaska. Recent work (2016-2019) has uncovered the tight coupling between climate, vegetation, and snow patterns, with important ramifications for permafrost condition. In the coming phase of the project, intensive field sites will be expanded to a broader region and will integrate with SnowEx and ABoVE studies to relate ground-based field data and remotely sensed information on snow and vegetation. The intensive field campaign and resulting analysis and modeling will inform improvement of the snow component of the Exascale Earth System Model Land Surface Model (E3SM-ELM) in Arctic regions.

Biogeochemical Sources and Exports in a Small Headwater Catchment Underlain with Discontinuous Permafrost

Nathan Conroy[1]*, Julian Dann[1], Brent Newman[1], Jeff Heikoop[1], Cathy Wilson[1], and Stan Wullschleger[2]

[1]Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM
[2]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: (nconroy@lanl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

High frequency surface water sampling was conducted at multiple locations along the main drainage of a small headwater catchment (2.25 km^2) located on the Seward Peninsula of Alaska that is underlain with discontinuous permafrost. The predominately southeast-facing hillslope is divided by a relatively deep catchment-drainage that flows perennially and also collects seasonal runoff from snowmelt and rain. As such, discharge varies significantly with season and numerous transitory seepages can be observed at certain times of the year. The main drainage also receives water from several relatively small branching tributaries. One of the larger tributaries (henceforth "the tributary") was monitored in this study because of its function as a natural culvert of overland flow, as well as clearly visible seepages from both organic and mineral layers. During the summers of 2016 and 2017, automated samplers were used to collect regular (24hrs 2016; 48hrs 2017) surface water samples from 2 locations along the main drainage (upstream and downstream) and 1 location along the tributary. Surface water pH, redox potential, and temperature were measured during sampler deployment in an effort to characterize "typical" geochemical conditions of the drainage and tributary. Surface water samples were monitored for major cations, major anions, and stable water isotopes. Precipitation (as snow and rain) was also collected and monitored for major cations, major anions, and stable water isotopes, when possible. The downstream automated sampler was co-located with a gaging station from a separate study, which made it possible to consider concentration versus discharge relationships of the catchment. Stable water isotopes indicate that the primary source of water to each sampling location was via long flow paths that provide ample time for meteoric waters to mix prior to reaching the main drainage. Nevertheless, it was clear that each location receives water from different sources. The upstream location receives water relatively high in sulfate and nitrate; the sulfate likely from oxidation of sulfidic minerals, while the source of nitrogen could be thawing permafrost, but is uncertain at this time. The stability of both sulfate and nitrate suggests persistently oxic subsurface conditions. The tributary location receives water relatively high in calcium, strontium, and magnesium; time versus concentrations trends suggests calcium and strontium are from a similar source and magnesium is from a dissimilar source. The downstream location shows clear indications of mixing between the upstream and tributary locations. A chemostatic/non-chemostatic concentration versus discharge analysis was conducted is presented within.

Integrating New Knowledge of Arctic Tundra Processes into DOE's E3SM Land Model

Peter Thornton[1*], Ben Sulman[1], Fengming Yuan[1], Scott Painter[1], Ahmad Jan[1], Jitu Kumar[1], Colleen Iversen[1], Verity Salmon[1], David Graham2, Stan Wullschleger[1], Cathy Wilson[3], Dylan Harp[3], Baptiste Dafflon[4], Margaret Torn[4], and William Riley[4]

[1]Environmental Sciences Division, Oak Ridge national Laboratory, Oak Ridge, TN
[2]Bioscience Division, Oak Ridge National Laboratory, Oak Ridge, TN
[3]Los Alamos National laboratory, Los Alamos, NM
[4]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: (thorntonpe@ornl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

We have identified multiple science areas where new process understanding developed through observation, experimentation, and synthesis can be integrated within the E3SM Land Model (ELM). These areas include improvements to the representation of hydrologic processes, improved representation of vegetation physiology and community ecology, and improved ability to understand and predict biogeochemical dynamics in systems with varying degrees of permafrost extent and thickness. Here we provide a summary of six targeted science areas, with roadmaps for connecting existing knowledge and ongoing research to model algorithms that are appropriate for representing Arctic tundra processes at the grid and sub-grid scales in a highly resolved Earth system model. Three ELM process developments relate to predictions of surface and subsurface hydrology in representative Arctic tundra landscape types. This work relies on aggregation of fine-scale modeling results up to scales of tens of meters to kilometers. We are extending this work to consider the dynamics of lateral transport and hillslope hydrology in more rugged terrain using intermediate scale models that characterize the structure and function of individual hillslopes or flow paths. We are further extending the spatial scope of this model integration effort to consider the interactions of terrain, vegetation, and wind patterns in the seasonal evolution of snowpack and its influence on soil moisture and temperature. We are also building new representative plant function types that capture the observed functional and structural variation in Arctic tundra vegetation, including new types for shrubs, herbaceous species, mosses, and lichens. This work includes the development and parameterization of special physiological traits such as nitrogen fixation in alder and low temperature acclimation for photosynthesis in multiple species. Finally, we are constructing a new representation of subsurface biogeochemical reaction and transport that integrates a mechanistic representation of redox chemistry with predictions of pH, organic matter distribution, and microbial populations and functional groups. The improved soil biogeochemistry reaction networks are being constrained by laboratory incubation studies and field observations. The resulting prediction framework is being tested as a module within ELM, and as a reaction capability for finer-scale models, operating in both cases through a common interface. We demonstrate early results and show various model evaluation metrics being used to assess improvement in prediction skill for different processes at different scales.

Leveraging Multi-Scale Remote Sensing to Improve our Understanding of Arctic Vegetation Diversity, Structure and Function

Shawn P. Serbin[1*], Daryl Yang[1], Andrew McMahon[1], Wouter Hantson[2], Bailey Morrison[1], Dan Hayes[2], Latha Baskaran[3], Verity Salmon[4], Amy Breen[5], Charles Miller[3], Sebastien Biraud[6], Kim Ely[1], and Alistair Rogers[1]

[1]Brookhaven National Laboratory, Upton, NY
[2] University of Maine, Orono, ME
[3]Jet Propulsion Laboratory, Pasadena, CA
[4]Oak Ridge National Laboratory, Oak Ridge, TN [5]University of Alaska Fairbanks, Fairbanks, AK [6]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: (sserbin@bnl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

Rapid warming in the Arctic is driving changes in vegetation distribution, structure, and function, with widespread implications for energy balance and biogeochemical cycling of the high latitude ecosystems. These changes can in turn affect regional to global climates through their changes to snow cover, albedo, carbon, water, and energy cycling. An improved understanding of plant composition and functional properties in the Arctic is therefore critical to predict the consequences of climate change, but it is currently lacking. Moreover, a predictive understand of Arctic ecosystems is limited by a lack observational data, and the resulting inadequate representation of plant trait variation across space and time drives large uncertainties in Earth system models (ESMs). An approach is needed to bridge the scales between detailed *in- situ* observations in remote locations and the larger, landscape context needed to inform ESMs on plant composition, structure, and function. In particular we lack how details on plant responses to biotic and abiotic drivers, such as climate, soils, topography, and disturbance.
Remote sensing data acquired from various platforms (e.g. near-surface, unmanned aerial system (UAS), airborne, and satellite) are critical for multi-scale monitoring of vegetation status and dynamics. Here we present our efforts to derive detailed maps of species composition, canopy structure, and functional traits from UAS platforms, and linked them up with large-scale airborne and satellite observations. We showed that our plot-to-pixel scaling approach can yield accurate models for predicting plant traits (i.e. R^2 between 0.50 and 0.89), though issues and considerations remain. Using UAS maps as a benchmark, we explored the spectral consistency across multi-scale remote sensing observations to identify issues related to scale and spectral mismatch that affect the upscaling of plant traits. We found that, within ecotypes, remote sensing data is generally comparable, but spatial variation in plant composition and structure, as well as plant patch size, drives the observed mismatch in spectral reflectance acquired from different platforms. Although we show that we can effectively scale up our measurements, we also highlight the challenges and call for approaches to address scale and sensor mis-match.

Distributed Temperature Profiling System for Improved Quantification of Soil Thermal and Physical Properties

Stijn Wielandt[1]*, Carlotta Brunetti[1], Patrick McClure[1], Ian Shirley[1], Sam Pullman[1], John Fitzpatrick[1], Hunter Akins[1], Jack Lamb[1], Sebastian Uhlemann[1], John Peterson[1], Baptiste Dafflon[1], and Susan Hubbard[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA Contact: (stijnwielandt@lbl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger
BER Program: TES Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov/

Insight into subsurface storage and fluxes of water, carbon and nutrients in permafrost environments is essential to understand and predict how Arctic ecosystems will change under warming temperatures. While the characterization and monitoring of thermal regimes and soil physical properties (including the fraction of soil constituents) is critical for improving the predictive understanding of heat and water fluxes across the landscape, conventional measurement approaches do not deliver sufficient spatiotemporal resolution and coverage. This research focuses on the design, development, deployment and use of an innovative Distributed Temperature Profiling (DTP) system, consisting of a large number of wireless vertically-resolved temperature probes to improve the estimation of soil physical properties, and heat and water fluxes in the subsurface and in snowpack. Leveraging on technological advancements in the field of ultra-low power integrated circuits, sensors and communication systems, we developed a low- cost and ultra-low-power DTP system for large scale deployments with unprecedented spatial density. The system has been deployed at about 100 locations in the NGEE-Arctic Teller watershed located on the Seward Peninsula (Alaska), which is characterized by discontinuous permafrost and high spatial variability of soil thermal and physical properties. The synchronously measured vertically-resolved temperature data in the snowpack and in the subsurface enable new insights into the control of snowpack on soil temperature, as well as the interactions between soil-topography-vegetation properties and thermal regimes across the watershed. In addition, we developed a Bayesian inversion approach based on a Markov chain Monte Carlo algorithm to estimate soil thermal properties (i.e., thermal diffusivity) from the DTP soil temperature time-series. Synthetic and field studies are performed to investigate the required natural variability in soil temperature for a successful estimation of thermal diffusivity and related physical properties at various depths. In future developments, LoRa communication capabilities for real-time ultra-low-power data transmission will be added to the DTP system, enabling automated integration with physically-based models and remote sensing data for watershed wide high-resolution prediction of heat, water and carbon fluxes.

Modeling the Impacts of Tundra Fire on Shrub Expansion

Zelalem A. Mekonnen[1*], William J. Riley[1], Robert F. Grant[2]

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

Contact: (zmekonnen@lbl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE project
Project Website: https://ngee-arctic.ornl.gov/

Observations show that the productivity and composition of high-latitude vegetation are changing in response to climate warming. Among these changes, the expansion of woody shrubs across the Arctic tundra has been widely reported. With rapid climate warming tundra fire is also reported to be more frequent and intense. The impact of these recent and predicted changes in fire regimes on shrub expansion is uncertain. Here, we applied a well-tested mechanistic ecosystem model, *ecosys*, to examine how tundra fire affects the productivity of shrubs. At site scale, the model was prescribed with known fire vs. non-fire (control) events across the selected sites in Kougarok watershed, Seward Peninsula, Alaska. At regional scale, we applied the model to examine the effects of the past and projected changes in fire regimes across the tundra ecosystems of Alaska. Our model result shows that tundra fire (1) alters surface vegetation, soil organic carbon stocks, seedbed quality, and thus seedling regeneration, (2) deepens the active layer, and (3) enhanced mineralization. We show that these processes control post-fire soil temperature, nutrient cycling, and competition among tundra plant functional types. We modeled a 21st century increase in shrub productivity in both simulations (with and without fire). Compared to control simulations, fire events were modeled to cause a decline in the spatial average NPP of shrubs (~11%) across Alaskan tundra. However, fire events were modeled to result in changes in the composition of the tundra plant functional types that particularly favors deciduous shrubs. We conclude that changes in vegetation composition, accelerated by fire events, have important implications to Arctic tundra ecosystem function through its effect on the carbon cycle and energy balance and thus on the climate system.

NGEE Arctic Phase 3 Project Management Priorities

Susan Heinz[1*] and Stan Wullschleger[1]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN Contact:

(heinzsl@ornl.gov)
Project Lead Principle Investigator (PI): Stan Wullschleger BER Program: TES
Project: NGEE Arctic
Project Website: https://ngee-arctic.ornl.gov

The Next-Generation Ecosystem Experiments (NGEE Arctic) is a 10-year project (2012 to 2022) to improve our predictive understanding of carbon (C)-rich Arctic system processes and feedbacks to climate. This is achieved through experiments, observations, and synthesis of existing datasets that strategically inform model process representation and parameterization, and that enhance the knowledge base required for model initialization, calibration, and evaluation.
As the project team moves forward with Phase 3 of the project (2020 to 2022), there are significant milestones that our project management plan addresses to make progress on deliverables. These include Integrated Modeling to support the DOE Energy Exascale Earth System Model (E3SM), Data Management to support the transfer of data and metadata holdings to the ESS-DIVE and continued safety management and safety culture awareness for field research activities. This poster will provide a summary of progress toward major Phase 3 milestones, risk management, lessons learned and future scope adjustments as we move toward project closure in 2022.

Terrestrial Ecosystem Science

Next Generation Ecosystem Experiments (NGEE): Tropics

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

Jeffrey Chambers[1*] (PI), Deb Agarwal[1], Stuart Davies[2], Rosie Fisher[3], Kolby Jardine[1], Michael Keller[4], Charles Koven[1], Lara Kueppers[1], Ruby Leung[5], Nathan McDowell[5], Alistair Rogers[6], Charuleka Varadharajan[1], Anthony Walker[7], Jeffrey Warren[7], Chongang Xu[8]

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

Contact: (jchambers@lbl.gov)
Project Lead Principal Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov

Project Abstract: 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. In support of BER's mission to advance a predictive understanding of Earth's climate and environmental systems, the Next Generation Ecosystem Experiments (NGEE)- Tropics aims to develop an improved predictive understanding of tropical forests and Earth system feedbacks to changing environmental drivers over the 21st Century. A strong synthetic coupling of modeling and experiment-observational methods (i.e. ModEx) is our fundamental approach toward attaining this goal, with our grand deliverable a representative, process-rich tropical forest ecosystem model, extending from bedrock to the top of the vegetative canopy- atmosphere interface, in which the dynamics and feedbacks of tropical ecosystems in a changing climate can be modeled at the scale and resolution of a next generation ESM grid cell.

Our work in Phase 1 revealed several high-priority areas for model development, evaluation, and parametrization, leading to the identification of three Research Focus Areas (RFAs) for Phase 2 that will advance understanding and model representation of processes at the individual (RFA1), community to regional (RFA2), and regional and global (RFA3) scales in E3SM-FATES. The science within these RFAs is organized into ModEx Work Packages (WP). Each WP is tightly coupled to existing model code within DOE's Energy Exascale Earth System Model (E3SM)-FATES, or focused on developing new process representation in the model. The WPs within each RFA are coordinated to enable the delivery of RFA-level goals for FATES development and evaluation.

E3SM-FATES is the unifying platform at the center of this organizational structure, providing integration of scientific advances across all three RFAs, and ultimately enabling the NGEE-Tropics team to address our key science questions. This RFA and WP structure along with our comprehensive ModEx approach NGEE-Tropics Phase 2 also allows testing of scientific hypotheses and reduction of uncertainty in emergent model outcomes for our RFA Science Questions.

Title: Identifying plant resource acquisition and allocation strategies for nutrient-enabled ELM-FATES

Elizabeth Agee*,[1] Ryan Knox,[2] Charlie Koven,[2] Rosie Fisher,[3] Stuart Davies,[4] and Anthony P. Walker[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Lawrence Berkeley National Laboratory, Berkeley, CA;
[3]CERFACS, Toulouse, France; and [4]Smithsonian Tropical Research Institute, Washington, DC

Contact: (ageela@ornl.gov)
Project Lead Principle Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: http://ngee-tropics.lbl.gov

Project Abstract: The ability of global models to correctly partition carbon inputs between biomass pools is critical for determining carbon residence time and capturing global carbon cycle dynamics. The allocation of biomass to leaf, stem, and root is intimately linked to the acquisition of key resources needed to support plant function. Within a community, there exist numerous strategies for acquiring and allocating resources, operating within developmental and competitive spaces, that ultimately shape the structure and function of ecosystems over long time scales. Of particular interest are the resource acquisition and allocation strategies of tropical forests—with soil nutrient concentrations (nitrogen and phosphorous) hypothesized to influence primary production and regulate forest growth. Size-structured or cohort-based models provide the means to test hypothesized allocation and acquisition strategies and quantify the impacts of the costs and benefits of these strategies on co-existence under resource limitation. We examined the current implementation of nutrient acquisition and carbon allocation schemes across a range of size-structured models (e.g., ELM-FATES, ED2, LPJ-GUESS) to assess the current state of the science and connect these efforts with current knowledge of plant functional strategies for resource acquisition and allocation. Framing acquisition and allocation along axes of costs and benefits, we identify multiple strategies to aid in the simulation of trait diversity and coexistence found in tropical forests along resource gradients. The results of this work will be used to propose future model developments and hypotheses which may be tested within the context of the larger NGEE-Tropics project.

Title: Determining the Best-Fit Model for Tropical Soil Phosphorus Sorption with Relevance to Earth System Models

Julia Brenner,[1]* Melanie A. Mayes,[1] Xiaojuan Yang,[1] Anthony Walker,[1] Jana R. Phillips,[1] Wyn Zenni,[1,2] Erika Marín-Spiotta[3]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Environmental Studies Program, Vassar College, Poughkeepsie, NY;
[3]Department of Geography, University of Madison-Wisconsin, Madison, WI

Contact: (brennerjm@ornl.gov)
Project Lead Principle Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract:
Low phosphorus (P) availability in tropical soils is thought to limit forest productivity. These soils often have high sorptive capacities due to high contents of clay particles and iron (Fe) and aluminum (Al) oxides, which form strong bonds with orthophosphate (PO_4^{3-}). Improving the understanding of soil sorptive characteristics will help Earth system models (ESMs) better estimate plant nutrient availability and the productive capacity of tropical forests. Sorption isotherms have been widely described using the Michaelis-Menten type Langmuir equation, particularly because it provides readily-interpretable parameters, such as the maximum sorption capacity (*Qmax*) of the soil. *Qmax* values are typically quite large, often reaching values >1000 mg PO_4-P per kg of soil (mg/kg). Non-agricultural tropical forests are unlikely to be exposed to this much PO_4, so the high values of the *Qmax* do little to describe soil P sorption dynamics at lower concentrations which represent more realistic amounts soil solution P. We conducted 41 equilibrium batch isotherm experiments, covering 8 soil series within 4 soil orders from Puerto Rico, using concentrations of P ranging from 0 to 1000 mg PO_4-P per L. Isotherms were quantified by fitting the data to both Langmuir and Freundlich (power-law) equations. At the low end of the isotherm, where 7 to 40 mg PO_4-P/L was added to the soils, the Langmuir equation greatly underestimated the amount of P sorbed to the soil, which translates to an overestimate of the bioavailability of P. In contrast, the Freundlich equation consistently provided an accurate estimate of bioavailability at low concentrations of added P. Our initial findings indicate that the Freundlich equation provides more realistic estimates of the soil P sink. The Freundlich equation would therefore provide more accurate representation of tropical-soil P sorption in ESMs that aim to project soil P interactions moving forward.

Title: **Modeling water available to plants to improve understanding of tropical forest response to drought and land use land cover change**

Yilin Fang*, Yanyan Cheng, Ruby Leung

Pacific Northwest National Laboratory, Richland, WA

Contact: (yilin.fang@pnnl.gov)
Project Lead Principal Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract:
Improving modeling of water available to plants is important for understanding how tropical forest responds to land use land cover change and drought. Here we present two parallel efforts to understand the processes that control the water available to plants. The first effort focuses on improving modeling of lateral processes, which have important effects on groundwater table and soil moisture, with consequential impacts on water available to plants and their response to drought. Land surface models such as E3SM Land Model (ELM) represent surface and subsurface hydrologic processes using a vertical column so lateral processes must be parameterized. To facilitate the development of parameterizations of lateral processes and to provide a benchmark for the parameterizations, ELM is being coupled to ParFlow so that hillslope scale hydrology can be represented in ELM. ParFlow is called from ELM through an external model interface. Data transfer between the two models is realized using mapping files in order to resolve the different domain decomposition approaches used in ELM and ParFlow for parallel computing. Simulations will be performed using ELM and ELM-ParFlow over the Amazon basin to assess the soil moisture and groundwater table depth and how they are modulated by surface heterogeneity and plant hydraulics in the basin. In a parallel effort to improve modeling of tropical forest response to land use land cover change, flux tower data from Agua Salud are used to parameterize C4 grass in FATES to improve modeling of the water and carbon dynamics of C4 grass. Numerical experiments are being performed using ELM-FATES to simulate the impacts of land cover change from mature forest to C4 grass and forest clear-cut. Analysis will be presented to evaluate the impact on seasonal water and carbon cycle dynamics in Agua Salud, with a particular focus on how land cover changes modulate the water available to plants and the interactions between water and carbon cycle processes.

Title: **Vertical and horizontal distributions of tree density, tree size, crown size and crown packing over the Brazilian Amazon from airborne lidar data**

Antonio Ferraz[1,2], Michael Keller[1,3,4], Marcos Longo[1], Jean Ometto[5], Sassan Saatchi[1,2]

[1]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA
[2] Institute of the Environment and Sustainability, University of California, Los Angeles, CA
[3]USDA-Forest Service International Institute of Tropical Forestry, San Juan, PR
[4] Embrapa Agricultural Informatics, Campinas, SP, Brazil
[6] National Institute for Space Research (INPE), São José dos Campos, SP, Brazil

Contact: (antonio.a.ferraz@jpl.nasa.gov)
Project Lead Principal Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract:
Tropical trees adapt the shape and size of their crowns in response to highly competitive environmental variations. Tree density and crown packing regulate light penetration and forest proprieties such as biological diversity, growth, competition, mortality and recruitment. It has been suggested that tropical tree crowns are extremely heterogeneous as canopy packing efficiency critically depends on the biological diversity and on within-species crown plasticity. Natural and anthropogenic disturbances (e.g. lightning, logging) also play a major role on tree demography and tree crown diversity. However, our knowledge of the relationship between canopy structure and the tropical ecosystems function is limited. Field measurements provide important data on tree diversity and demographics but measurements of three-dimensional forest structure from the ground are difficult and scarce.
Using extensive airborne lidar data, we extracted individual tree crowns (Ferraz et al., 2016) from 470 samples (6.25ha) located in *terra firme* forests within the Brazilian Amazon. The samples were selected from a collection 558 transects (15 km x 0.5km) of airborne lidar data acquired in 2016 in a random design.
We examined patterns of tree density and crown packing across gradients of forest cover, soils topography and climate. Specifically, we compare intra-plot and inter-plot variability in tree density, tree size (height and crown dimensions), tree competition, crown packing, and crown plasticity. By analyzing the lidar derived three-dimensional crowns maps, we test whether increased canopy packing primarily occurs through vertical stratification or horizontal space filling. We use coincident field inventory over a limited number of sites to study the response of species richness to tree competition, crown packing and plasticity.
Our datasets provide a unique Amazon-scale tree crown structural benchmark to study role of forest structure biogeochemical and climatic processes. Chronosequence analyses (e.g. time since last disturbance) enable the study of competing plant functional traits that drive vertical and/or horizontal crown packing, govern forest light conditions and favor forest regenaration and carbon storage.

Title: Benchmarking and Parameter Sensitivity of Physiological and Vegetation Dynamics using the Functionally Assembled Terrestrial Ecosystem Simulator (FATES) at Barro Colorado Island, Panama

Charlie Koven,[1] et al.

[1]Lawrence Berkeley National Lab, Berkeley, CA, USA

Contact: (cdkoven@lbl.gov)
Project Lead Principal Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov

Project Abstract: Plant functional traits determine vegetation responses to environmental variation, but variation in trait values is large, even within a single site. Likewise, uncertainty in how these traits map to Earth system feedbacks is large. We use a vegetation demographic model (VDM), the Functionally Assembled Terrestrial Ecosystem Simulator (FATES), to explore parameter sensitivity of model predictions, and comparison to observations, at a tropical forest site: Barro Colorado Island in Panama. We define a single 12-dimensional distribution of plant trait variation, derived primarily from observations in Panama, and define plant functional types (PFTs) as random draws from this distribution. We compare several model ensembles, where individual ensemble members vary only in the plant traits that define PFTs, and separate ensembles differ from each other based on either model structural assumptions or non-trait, ecosystem-level parameters, which include: (a) the number of competing PFTs present in any simulation, and (b) parameters that govern disturbance and height-based light competition. While single-PFT simulations are roughy consistent with observations of productivity at BCI, increasing the number of competing PFTs strongly shifts model predictions towards higher productivity and biomass forests. Different ecosystem variables show greater sensitivity than others to the number of competing PFTs, with the predictions that are most dominated by large trees, such as biomass, being the most sensitive. Changing disturbance and height-sorting parameters, i.e. the rules of competitive trait filtering, shifts regimes of dominance or coexistence between early and late successional PFTs in the model. Increases to the extent or severity of disturbance, or to the degree of determinism in height-based light competition, all act to shift the community towards early-successional PFTs. In turn, these shifts in competitive outcomes alter predictions of ecosystem states and fluxes, with more early-successional dominated forests having lower biomass. It is thus crucial to differentiate between plant traits, which are under competitive pressure in VDMs, from those model parameters that are not, and to better understand the relationships between these two types of model parameters, to quantify sources of uncertainty in VDMs.

Title: Quantifying Phenological Variations in Tropical Forests Across Scales Using High Spatio-Temporal Satellite Remote sensing

Jitendra Kumar and Forrest M. Hoffman

Oak Ridge National Laboratory

Contact: (kumarj@ornl.gov)
Project Lead Principle Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract: Vegetation phenology is an integrated and sensitive indicator of ecosystem function that responds to disturbance, seasonality, variability and extremes in weather and climate change. Vegetation phenology modulates the surface energy balance and hydrological processes at the landscape scale. Understanding of tropical forest phenology however is limited, due to high diversity of tree species exhibiting a variety of phenological patterns. Heterogeneous tropical forests also exhibit highly variable and heterogeneous responses to the biotic and abiotics stressors. Satellite remote sensing has been long used to study vegetation phenology. However, frequent cloud cover, smoke from fire, and sensor artifacts complicates the satellite based study of land surface phenology. Widely used satellite platforms like MODIS and Landsat suffer from the limitation over coarse spatial resolution or lack of temporal repeat frequency, this limiting their ability to provide detailed understanding of heterogeneous phenological patterns on the landscape. However, increasing availability of high spatial and temporal resolution remote sensing data offer new opportunities to study tropical tree phenology and understand the role of diversity and heterogeneity across spatial scales of a Flux tower to the landscape. In this study we used satellite remote sensing data from VENµS, an cooperative Earth observation program of Israel and France is a mini-satellite with scientific mission of terrestrial environment monitoring, to study phenology. We acquired and processed data, at 10m spatial resolution, VENµS at a number of FlUXNET sites in Panama and Amazon during 2017-2019. While the satellite captures data at every other day interval, the number of usable cloud free images, while limited, still provides an new insight in the temporal variability in vegetation phenology at high resolution. Analysis of these data sets along with those from MODIS and Sentinel-platforms near selected FLUXNET sites also help quantify and understand the multi-scale nature of phenology and role of diversity and heterogeneity. In this poster, we will share results from our ongoing analysis of tropical forest phenology using multi-source remote sensing data at varying spatial and temporal resolution.

Title: **Representing Subsurface Lateral Groundwater Flow in Earth System Models**

Chang Liao*, Ruby Leung, Yilin Fang, Teklu Tesfa

Pacific Northwest National Laboratory

Contact: (chang.liao@pnnl.gov)
Project Lead Principal Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract:
Subsurface lateral groundwater flow plays an important role in controlling water table dynamics. Due to the relatively coarse spatial resolutions of land surface and Earth system models, this process is often omitted even though it can be significant due to subgrid heterogeneity. In this study, we developed a physically based model, Hydrological Hillslope Soil Column (H2SC), to simulate subsurface lateral groundwater flow using hillslopes to represent subgrid spatial variability in topography. This model explicitly considers the transitions between different water table scenarios (e.g., with or without a seepage phase) and the interactions between land and river. We coupled this model to the land component (ELM) and river component (MOSART) of the Energy Exascale Earth System Model (E3SM) and applied it globally. H2SC is being calibrated using observed water table depth. Model evaluation will be performed using observational data of the surface water balance. Preliminary simulations show that lateral groundwater flow is affected by topography through its impacts on water table slopes. Analysis will be performed to understand how lateral flow contributes to the river discharge and influences the spatial distributions of water table along the hillslope.

Title: Landscape controls of biomass accumulation in second growth tropical forests after agricultural abandonment

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

[1]SILVIS Lab, University of Wisconsin, Madison, WI 53706, USA
[2]NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA
[3]USDA Forest Service International Institute of Tropical Forestry, San Juan, PR 00926, USA
[4]Jet Propulsion Laboratory, Pasadena, CA 91109, USA
[*]Corresponding author

Contact: (martinuzzi@wisc.edu)

Project Lead Principal Investigator (PI): Jeff Chambers, LBNL

BER Program: TES

Project: NGEE-Tropics

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

Project Abstract:
Understanding the landscape controls of biomass accumulation in second-growth tropical forests is key for understanding the global carbon cycle and advancing earth system modeling. We present an update on our study assessing rates and controls of biomass accumulation following land use abandonment, using Puerto Rico as a case study. We integrated a lidar-based biomass map with information on forest age, past land use, substrate, topography, and climate. We found that aboveground biomass accumulated rapidly in the first ~30 years, but thereafter accumulated more slowly, and with substantial variability. Time since abandonment in combination with the type of past land use and topographic position influence biomass accumulation. We present our results from multiple perspectives including summary statistics, parametric, and non-parametric (random forests) multivariate analyses. Information from our study will be valuable to parametrize processes of forest biomass accumulation in Earth System Models such as E3SM-FATES.

Title: **Pervasive shifts in forest dynamics in a changing world**

Nate G. McDowell[1*], Craig D. Allen[2], Kristina Anderson-Teixeira[3,4], Brian H. Aukema[5], Ben Bond- Lamberty[6], Louise Chini[7], James S. Clark[8], Michael Dietze[9], Charlotte Grossiord[10], Adam Hanbury- Brown[11], George C. Hurtt[7], Robert B. Jackson[12], Daniel J. Johnson[13], Lara Kueppers[11,14], Jeremy W. Lichstein[13], Kiona Ogle[15], Ben Poulter[16], Thomas A.M. Pugh[17], Rupert Seidl[18,19], Monica G. Turner[20], Maria Uriarte[21], Anthony P. Walker[22], Chonggang Xu[23]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]US Geological Survey, Los Alamos, NM; [3]Smithsonian Conservation Biology Institute, Front Royal, VA; [4]Smithsonian Tropical Research Institute, Panama; [5]University of Minnesota, St. Paul, MN; [6]Joint Global Change Research Institute, Pacific Northwest National Laboratory, College Park, MD; [7]University of Maryland, College Park, MD; [8]Duke University, Durham, NC; [9]Boston University, Boston, MA; [10]Swiss Federal Institute for Forest, Snow and Landscape Research WSL, Switzerland; [11]University of California-Berkeley, Berkeley, CA; [12]Stanford University, Stanford, CA; [13]University of Florida, Gainesville, FL; [14]Lawrence Berkeley National Laboratory, Berkeley, CA; [15]Northern Arizona University, Flagstaff, AZ; [16]NASA Goddard Space Flight Center, Greenbelt, MD; [17]University of Birmingham, Birmingham, UK; [18]University of Natural Resources and Life Sciences, Vienna, Austria; [19]Technical University of Munich, Freising, Germany; [20]University of Wisconsin-Madison, Madison, WI; [21]Columbia University, New York, NY; [22]Oak Ridge National Laboratory, Oak Ridge, TN; [23]Los Alamos National Laboratory, Los Alamos, NM

Contact: (nate.mcdowell@pnnl.gov)
Project Lead Principal Investigator (PI): Jeff Chambers (NGEE-Tropics); Jim Clark and Lara Kueppers for the DOE workshop "Disturbance and vegetation dynamics in Earth System Models in March 2018.
BER Program: TES
Project: NGEE-Tropics, and the DOE workshop "Disturbance and vegetation dynamics in Earth System Models in March 2018.
Project Website: https://ngee-tropics.lbl.gov/;
https://tes.science.energy.gov/workshops/vegetationdynamics.shtml

Project Abstract: Forest dynamics arise from the interplay of chronic drivers and transient disturbances with the demographic processes of recruitment, growth, and mortality. The resulting trajectories of vegetation development drive the biomass and species composition of terrestrial ecosystems. Forest dynamics are changing due to anthropogenic-driven exacerbation of chronic drivers, such as rising temperature and CO_2, and increasing transient disturbances, including wildfire, drought, windthrow, biotic attack, and land-use change. There are widespread observations of increasing tree mortality due to changing climate and land use, accompanied by observations of growth stimulation of younger forests due to CO_2 fertilization. These antagonistic processes are co-occurring globally, leaving the fate of future forests uncertain.

We examine the implications of changing forest demography and its drivers as a critical uncertainty for both future forest management and forecasting impacts of global climate forcing. Ongoing changes in environmental drivers and disturbance regimes are consistently increasing mortality and forcing forests towards shorter and younger stands, reducing potential carbon storage. Acclimation, adaptation, and migration may partially mitigate these effects. These increased forest impacts are due to natural disturbances (e.g. wildfire, drought, windthrow, insect/pathogen outbreaks) and land-use change, both of which are predicted to increase in magnitude in the future. Tree growth, and potentially recruitment, may have increased globally in the 20th century based on atmospherically derived estimates of the terrestrial carbon sink and based on remote sensing data, but the growth of this carbon sink has slowed. Variability in growth stimulation due to CO_2 fertilization is evident globally, with observations and experiments suggesting that forests benefit from CO_2 primarily in early stages of secondary succession. Furthermore, increased tree growth typically requires sufficient water and nutrients to take advantage of rising CO_2. Collectively, the evidence reveals that it is highly likely that tree mortality rates will continue to increase while recruitment and growth will respond to changing drivers in a spatially and temporally variable manner. The net impact will be a reduction in forest canopy cover and

biomass.

Pervasive shifts in forest vegetation dynamics are already occurring and are likely to accelerate under future global changes, with consequences for biodiversity and climate forcing. The emergent hypotheses are testable using emerging terrestrial and satellite-based observation networks. The existing evidence and new observations provide a critical test of Earth system models that continue to improve in their ability to simulate forest dynamics and resulting climate forcing.

Title: First soil-specific calibrated measurements of soil moisture in a Central Amazonian tropical forest

Robinson Negrón-Juárez[1*], Savio J. F. Ferreira[2], Marcelo Crestani Mota[2], Boris Faybishenko[1], Maria Terezinha F. Monteiro[2], Luiz A. Candido[2], Rubia Pereira Ribeiro[2], Regison Costa de Oliveira[2], Alessandro C. de Araujo[3], Jeffrey M. Warren[4], Brent D. Newman[5], Bruno O. Gimenez[2], Charuleka Varadharajan[1], Deborah Agarwal[1], Laura Borma[6], Javier Tomasella[7], Niro Higuchi[2], Jeffrey Q. Chambers[1]

[1] Lawrence Berkeley National Laboratory, Berkeley, CA, USA;
[2] Brazil's National Institute for Amazonian Research, Manaus, Brazil;
[3] Brazilian Agricultural Research Corporation, Para, Brazil;
[4] Oak Ridge National Laboratory, Oak Ridge, TN, USA;
[5] Los Alamos National Laboratory, Los Alamos, NM, USA;
[6] Brazil's National Institute for Space Research, Sao Paulo, Brazil
[7] National Center for Monitoring and Alerts for Natural Disasters, Sao Paulo, Brazil

Contact: robinson.inj@lbl.gov
Project Lead Principle Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract: Soil moisture plays a key role in hydrological, biogeochemical and energy budgets, which means that accurate soil moisture measurements are required to characterize and model feedbacks between these three systems and to quantify fluxes and processes. Accurate soil moisture measurements are difficult because of logistical constraints in remote areas such as the Amazon. In this study, we evaluated the need for field based calibration of time domain reflectometers (TDR) for moisture content measurements in tropical forest soils. We also present soil moisture data time series from a deep soil profile in an undisturbed forest at the ZF2 field site near Manaus, Brazil. High resolution time series of soil moisture in tropical forests are limited, especially in the central Amazon, and most of the tropical soil moisture data that are available have been collected from shallow soils (typically < 1 m). An unusual aspect of this study is that it examines soil moisture across wet- and dry-seasons in a tropical forest down to nearly 15-m depth. Comparison of TDR calibrations between the widely used general or "factory" calibration based on the Topp equation and a third degree polynomial calibration based on dielectric permittivity and moisture content measurements from local pit soils showed substantial differences. We found that the general TDR equation underestimated volumetric moisture contents (θ_v) by 22-42%. The calibration using local soils to quantify the TDR permittivity-water content relation was much more accurate. The magnitude of the differences between the calibration approaches suggests that use of the general equation may result in significant error when applied to humid tropical forest soils. The calibrated wet- and dry-season θ_v data showed a variety of depth and temporal variations highlighting the importance of soil textural changes, root uptake depths, as well as event- to seasonal-precipitation effects. Data such as these are greatly needed for improving our understanding of ecohydrological processes within tropical forests and for improving models of these systems in the face of changing environmental conditions.

Title: **Quantifying Soil Percolation Dynamics & Biogeochemical Transport in Tropical Soils near Manaus, Brazil**

Brent D. Newman[1*], Jardel Rodrigues[2], Bruno Gimenez[2,6], Adam Collins[1], Jeff Warren[3], Niro Higuchi[2], Savio Ferreira[2], Robinson Negron-Jaurez[4], Kolby Jardine[4], Ruby Leung[5], Chonggang Xu[1]

[1]Earth & Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM
[2]National Institute of Amazonian Research (INPA), Manaus, AM, Brazil
[3]Oak Ridge National Laboratory, Oak Ridge, TN [4]Lawrence Berkeley National Laboratory, Berkeley, CA [5]Pacific Northwest National Laboratory, Richland, WA [6]now at Smithsonian Tropical Research Institute (STRI)

Contact: bnewman@lanl.gov

Project Lead Principle Investigator (PI): Jeff Chambers, LBNL

BER Program: TES

Project: NGEE-Tropics

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

Project Abstract:
Understanding soil moisture dynamics & associated transport of biogeochemical species is challenging in tropical systems because of the physical nature of tropical soils and the coupled ecohydrological impacts on flow & transport. We utilized an unusual type of passive wick flux meter (or drainage lysimeter) to measure real-time percolation fluxes & to sample percolation chemistry & stable isotopes along two topographic transects at the ZF2 field area near Manaus, Brazil (Rodrigues et al., 2019). Percolation flux is often an inferred or modeled process & as such has significant uncertainties especially in forested soils where preferential flow paths are often important. Direct continuous measurement of fluxes provides a way to inversely calibrate hydrological model parameters which should yield more representative simulations of actual field conditions. In addition, by coupling percolation flux measurements with biogeochemistry we can understand transport dynamics of nutrients and other geochemical species. Results indicate that percolation is frequent on a daily basis, occurring 63%, 73%, & 79% of the time in the plateau, slope & valley locations, respectively. It is also highly pulsed & varies greatly with rainfall amount & season. Overall temporal percolation patterns are similar in the three topographies, but the amounts of percolation vary substantially and cumultative percolation flux was found to be greatest in the valleys, intermediate on the slopes, and lowest on the plateaus.
Percolation water biogeochemistry also varies with space & time. Nitrate concentrations are extremely high at all locations. Stable isotope results indicate microbial nitrate production, but with substantial denitrification events. Nitrogen appears unlikely to be a co-limiting nutrient in these forests. Phosphate concentrations are consistent with a phosphorus nutrient limitation.

Title: The LBA / NGEE-Tropics data collaboration and water dynamics impacts of the 2015 drought in Central Amazon

Gilberto Z. Pastorello[1], Robinson I. Negron-Juarez[1], Yao Tang[2], Kolby J. Jardine[1], Bruno O. Gimenez[3], Alessandro C. Araújo[4,5], Sávio J.F. Ferreira[5], Marta O. Sá[5], Paulo R. Teixeira[5], Leila S.M. Leal[5], Terezinha Monteiro[5], Luiz A. Candido[5], Stephen W. Chan[1], Charlie D. Koven[1], and Jeffrey Q. Chambers[1,6]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]Plummer Associates, Inc, Fort Worth, TX;
[3]Smithsonian Tropical Research Institute, Panama City, Panama;
[4]Embrapa Eastern Amazon, Belém, PA, Brazil;
[5]National Institute for Amazon Research (INPA), Large Scale Biosphere-Atmosphere Program (LBA), Manaus, AM, Brazil;
[6]University of California, Berkeley, CA.

Contact: (gzpastorello@lbl.gov)

Project Lead Principal Investigator (PI): Jeff Chambers, LBNL

BER Program: TES

Project: NGEE-Tropics

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

Project Abstract: The LBA Program operates a network of micrometeorology and hydrology field stations across the Amazon. In partnership with NGEE-Tropics, datasets from these stations are being QA/QC'd and prepared for synthesis studies and also as driving and validating measurements for FATES model runs. One of our joint studies is focusing on the ecosystem effects of the 2015-2016 El Niño, the second strongest since 1950s and with record-breaking effects causing a sharp decrease in precipitation and increase in temperature over tropical South America. While the spatial distribution of the 2015-2016 drought was unusual and concentrated into a smaller region in northeastern Amazonia, the ZF2 reserve near Manaus in the central Amazon was heavily impacted. Measurements of soil moisture, sap flow, and eddy-covariance fluxes, among other micrometeorological variables, collected at the ZF2 K34 tower (AmeriFlux ID BR-Ma2), clearly show the effects of this drought event. We explored these data looking for quantitative and mechanistic relationships between soil moisture, plant transpiration, and evapotranspiration. In this poster, we present results from our study with a quantification of soil water dynamics, plant transpiration, and forest evapotranspiration during the 2015 drought. We also discuss other ongoing and future work in the Amazon within the context of the LBA / NGEE-Tropics collaboration.

Title: Examining Hydraulic Safety Margins in the Context of Drought Mortality Rates

Alexandria L. Pivovaroff[1*], Nate McDowell[1], Brett T. Wolfe[2,3], Bradley Christoffersen[4], Stuart Davies[2], L. Turin Dickman[5], Charlotte Grossiord[6,7], Riley T. Leff[1], Alistair Rogers[8], Shawn P. Serbin[8], Cynthia Wright[9], S. Joseph Wright[2], Jin Wu[8,10], Chonggang Xu[5], Alfonso Zambrano[2], Jeffrey Q. Chambers[11]

[1]Pacific Northwest National Laboratory, Richland WA USA
[2]Smithsonian Tropical Research Institute, Balboa, Republic of Panama
[3]School of Renewable Natural Resources, Louisiana State University, Baton Rouge, LA, U.S.A.
[4]University of Texas Rio Grande Valley, Department of Biology, Brownsville TX USA
[5]Los Alamos National Laboratory, Los Alamos, NM USA
[6]Swiss Federal Institute for Forest, Snow and Landscape Research WSL, Forest Dynamics Research Unit, Birmensdorf, Switzerland
[7]École Polytechnique Fédérale de Lausanne EPFL, School of Architecture, Civil and Environmental Engineering ENAC, Switzerland
[8]Brookhaven National Laboratory, Upton NY USA
[9]Oak Ridge National Lab, Oak Ridge, TN USA
[10]School of Biological Sciences, The University of Hong Kong, Pokfulam Road, Hong Kong
[11]Lawrence Berkeley National Laboratory, Berkeley, CA USA

Contact: (alexandria.pivovaroff@pnnl.gov)

Project Lead Principle Investigator (PI): Jeff Chambers, LBNL

BER Program: TES

Project: NGEE-Tropics

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

Project Abstract:

Moist tropical forests are home to an estimated 50-60% of Earth's species and are responsible for about 50% of terrestrial gross primary productivity. However, climate change, including drought, is driving tree mortality and leading to forest degradation across the globe. We investigated if species' drought mortality rates were associated with plant hydraulic and water relations traits, including hydraulic safety margins, i.e. the extent to which plants buffer themselves from thresholds of water stress. To test this, we used long-term census data from ForestGEO to determine species-specific drought mortality rates across multiple sites in Panama. We then compared these drought mortality rates with hydraulic traits, including gas exchange, water potentials, turgor loss point, and hydraulic safety margins. Along a continuum of drought mortality rates, we found that drought vulnerable species were generally more light-demanding, while drought resistant species were generally more shade tolerant. However, initial results indicated that drought mortality rates were not coordinated with hydraulic traits, including hydraulic safety margins.

Title: **Process-Based Model Predictions of Tropical Forest Function Across a Precipitation Gradient in Panama.**

Thomas Powell[1], Chonggang Xu[2], Elmera Azadpour[1], Charles Koven[1], Lara Kueppers[1,3]

[1]Lawrence Berkeley National Laboratory, Berkeley, California, USA
[2]Los Alamos National Laboratory, Los Alamos, New Mexico, USA
[3]Energy and Resources Group, University of California, Berkeley, California, USA

Contact: (tlpowell@lbl.gov)

Project Lead Principal Investigator (PI): Jeff Chambers, LBNL

BER Program: TES

Project: NGEE-Tropics

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

Project Abstract:
Climate change over the coming century is likely to cause large and diverse impacts on plant available water (PAW) across many areas of the tropics. However, there is considerable uncertainty regarding how diverse tropical forest structure and function will respond to changes in PAW. Therefore, we used the Functionally Assembled Terrestrial Ecosystem Simulator (FATES) to assess how tropical forests may respond to PAW gradients caused by edaphic and precipitation variation. The three sites examined in this study cover a precipitation gradient across the Isthmus of Panama: Parque Nacional San Lorenzo (SLZ: c. 3000 mm yr^{-1}), Barro Colorado Island (BCI: c. 2600 mm yr^{-1}), and Parque Nacional Metropolitano (PNM: c. 1800 mm yr^{-1}). The three sites also differ in soil texture with clay contents of approximately 80%, 70% and 35% for SLZ, BCI, and PNM, respectively. Three different sets of simulations were performed with FATES to examine the effects site-level differences in meteorology and edaphic properties independently and jointly have on model predictions. The first set of three simulations used a common soil texture from BCI and meteorology from each site. The second set of three simulations used a common meteorology from BCI and soil textures from each site. The third set of three simulations used the meteorology and soil texture of each site respectively. Included in this analysis is a characterization of how locally measured precipitation, air temperature, and incoming radiation differs across the three sites. Model results explore how gross primary production (GPP), forest structure and composition, and aboveground biomass vary across the precipitation and edaphic gradients.

Title: Should Terrestrial Biosphere Models Remove Triose Phosphate Utilization Limitation from Their Representation of Photosynthesis?

Alistair Rogers[1], Dushan P. Kumarathunge[2], Danica L. Lombardozzi[3], Shawn P. Serbin[1] Belinda E. Medlyn[4], Anthony Walker[5]

[1]Environmental and Climate Sciences Department, Brookhaven National Laboratory, Upton, NY [2]Plant Physiology Division, Coconut Research Institute of Sri Lanka, Lunuwila, Sri Lanka [3]Climate and Global Dynamics Division, National Center for Atmospheric Research, Boulder, CO [4]Hawkesbury Institute for the Environment, Western Sydney University, Penrith, Australia [5]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: (arogers@bnl.gov)

Project Lead Principle Investigator (PI): Jeff Chambers (LBNL) & Stan Wullschleger (ORNL)

BER Program: TES

Project: NGEE-Tropics & NGEE Arctic

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

Project Abstract: Triose phosphates are the principal product of photosynthesis. They are utilized within the chloroplast for starch synthesis or translocated to the cytosol where they fuel sucrose synthesis. However, the limitation of photosynthesis by the triose phosphate utilization (TPU) rate can occur when the capacity for sucrose and starch synthesis are not sufficient to maintain a phosphate pool size that is capable of meeting the demand for ATP synthesis and the subsequent use of that ATP by the Calvin-Benson cycle. The Farquhar, von Caemmerer & Berry (FvCB) model of photosynthesis is at the heart of many terrestrial biosphere models (TBMs) that seek to understand the global carbon cycle and project the response of the terrestrial biosphere to global change. Several TBMs include representation of the TPU limited rate of photosynthesis as a potential limitation of photosynthesis. However, representation of TPU limitation in TBMs is currently based on an arbitrary relationship with the maximum carboxylation capacity. Furthermore, recent work has (1) demonstrated the sensitivity of TBM output to model representation of TPU, (2) revealed potential artifacts within some TBMs that exaggerate the impact of including formulations of TPU limitation, (3) showed that when measured under growth conditions TPU limitation rarely limits photosynthesis, even at low temperature. Collectively, these advances, suggest that current model formulations of TPU limitation should be removed from TBMs until we have an improved understanding and model representation of this process.

Title: Where do trees' source water during drought? Inverse modeling reveals drought strategies coordinating water-uptake depths with above ground traits

Rutuja Chitra-Tarak[1,2], Chonggang Xu[1], Laurent Ruiz[3,4,5], Matteo Detto[6], Brett Wolfe[7], Nobert Kunert[8], Kristina Anderson-Texeira[8,9], Brent Newmann[1], Lawren Sack[10], Joseph Zailaa[10] & SM McMahon[2,9]

[1]Earth and Environmental Science Division, Los Alamos National Laboratory, NM; [2]Smithsonian Environmental Research Center, Edgewater, MD; [3]Indo-French Cell for Water Sciences, Indian Institute of Science, Bangalore India; [4]UMR SAS, INRA, Rennes, France; [5]IRD, UMR, Université de Toulouse, CNRS, Toulouse, France; [6]Princeton University, Princeton, NJ; [7]Lousiana State University, Baton Rouge, LA; [8]Smithsonian Conservation Biology Institute, Front Royal, VA; [9]Smithsonian Tropical Research Institute, Gamboa, Panama; [10]University of California, Los Angeles, CA

Contact: (rutuja@lanl.gov)
Project Lead Principle Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: http://ngee-tropics.lbl.gov/

Project Abstract: Forests are critical to the terrestrial carbon and water cycle, but droughts are predicted to increase in frequency and intensity, threatening forest function through lower productivity and increased mortality. Identifying species differences in drought response is critical to predicting the extent of this threat. Species strategies for handling water stress have been explored almost entirely in terms of above-ground responses, but not how water stress might be avoided or tolerated through differential access to the highly dynamic below-ground water environment. This is especially challenging to study in tropical forests with hundreds to thousands of tree species. Here we present a first instance of a well-validated, inverse model that estimated trees' water-uptake depths scaled up to scores of co-existing tree species. We hypothesized that trees' growth dynamics was a function of a species' rooting profile (an unknown), and the dynamics of plant water potential along that profile plus an error term.

We tested this approach at the seasonally dry tropical forest of BCI, Panama by estimating rooting profiles for 51 tree species that best explained their 25 yearlong records of growth dynamics (1990-2015). To obtain reliable, concurrent estimates of water potential and plant available water throughout the rooting zone we locally parameterized DOE's Energy Exascale Earth System Model (E3SM) - Functionally Assembled Terrestrial Ecosystem Simulator (FATES). We calibrated it against observations of soil moisture dynamics by depth, evapotranspiration and stream runoff.

Forced with local climate data, we then ran ensemble simulations of E3SM-FATES over 1985-2015. We calculated species' mean water-uptake depths as a function of best-fit species-specific rooting profiles as well as water potential and plant available water in each soil layer up to 13 m.

The 51 species showed diverse water-uptake depths (0.1-13 m). For a subset of species with data on xylem sap ^2H concentration indicating their water-sourcing depths model matched data well. This match was especially better when we used species-specific Turgor Loss Point as the limit to water-uptake. We also found that species with deep water access were associated with drier sites within the plot, as well as, across the Isthmus of Panama, had larger Leaf Mass to Area ratio, higher leaf-level hydraulic conductivity, and larger safety margin based on capacitance. These results suggest that drought strategies of co-existing tree species are an integration of well-coordinated above- and below-ground traits suited to their different water environments.

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

Jacquelyn Shuman,[1*] Rosie Fisher,[1,2] Charlie Koven,[3] Ryan Knox,[3] Chonggang Xu,[4] and Sam Levis,[3]

[1]National Center for Atmospheric Research, Boulder, CO;
[2]Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS), Toulouse, France;
[3]Lawrence Berkley National Laboratory, Berkley, CA; and
[4]Los Alamos National Laboratory, Los Alamos, NM

Contact: (jkshuman@ucar.edu)
Project Lead Principle Investigator (PI): Jeff Chambers, LBNL
BER Program TES
Project: NGEET-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract: Within the tropics, fire acts to determine vegetation size distribution, biomass accumulation, and the dominance or coexistence of trees and grasses in part setting the forest- savanna biome boundary. This results from complex feedbacks and interactions between vegetation, fire, and climate. Tropical forests are a critical part of the global cycle for carbon and water, thus it is important to analyze how the interaction of climate and fire drive forest-savanna transitions. Utilizing the Functionally Assembled Terrestrial Ecosystem Simulator (FATES), a size-structured demographic vegetation model, with the fire behavior and effects module SPITFIRE we explore functional thresholds of trees and grass across the tropics with active fire disturbance. SPITFIRE is updated to include new fire behavior formulations for fire intensity, scorch height, fuel consumption and coarse woody debris fractions, as well as live grass fuel moisture dynamics based on climate, and the ability to read spatially and temporally varying lightning datasets. With these updates FATES-SPITFIRE captures observed interannual and seasonal burned fraction variability for the recent historical period. FATES-SPITFIRE tracks size-structured plant mortality during fire events and captures 'fire-trap' dynamics where trees escape fire by achieving a canopy height above the flames or through fire resistant traits. In simulations, fire limits tree extent, with wetter areas retaining a higher stable tree fraction under an active fire regime. Transitional and drier moisture zones across South America demonstrate dominance of trees or grasses conditional on vegetation traits and strategies, with more expensive traits leading to lower compositional dominance and biomass accumulation compared to similar plants. These results capture critical size-structured competitive interactions, degradation and loss. FATES-SPITFIRE demonstrates that it captures ecosystem assembly of forest- grassland transitions across moisture and disturbance gradients within the tropics through the fire-vegetation feedbacks that are critical for prediction of ecosystem resilience and shifts under current and future conditions.

Title: **Plant water sourcing in the neotropics—effects of topography and rainfall**

Cynthia Wright,[1*] Alex Pivovaroff,[2] Nate McDowell,[2] Brent Newman,[3] Jeff Warren,[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN; [*]presenting author; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Los Alamos National Laboratory, Los Alamos, NM;

Contact: (wrightcl1@orng.gov)

Project Lead Principle Investigator (PI): Jeff Chambers, LBNL

BER Program: TES

Project: NGEE-Tropics

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

Project Abstract: Plant water sourcing and rooting depth are critical in understanding and predicting tropical forest response to climate change scenarios—specifically how changes in the timing and availability of soil water influence net carbon exchange. Yet we know very little about tree rooting depths and how water extraction patterns vary by species, soil type, depth to water table, and degree of rainfall seasonality. To address this type of uncertainty, the E3SM-FATES land model was developed to represent the dynamics of tree cohorts of differing size and functional types, allowing for the representation of variable water extraction patterns. This modeling effort represents a major advancement in Earth systems models. Still, E3SM-FATES has not yet been parameterized and validated with field data. The objective of this research, therefore, is to quantify tree water sourcing and rooting depth as a function of species and across a topographic and hydrologic gradient. Preliminary results for a tropical rainforest near Manaus, Brazil show that fine roots distribution has strong correlation with rates of water uptake. Yet, a transition from wet to dry conditions indicates that water sources shift to deeper soil layers. Although fine root biomass declines with depth, during dry conditions, 30% or more of daily plant water use is extracted from the 1+ m depth. To quantify species-specific depth of water uptake during drying conditions, we are using vertical profiles of stable isotopes of water (δ^2H and δ^{18}O) within the soils and plants as natural tracers. Data are coupled with soil water content, sap flux and transpiration patterns. First, we are testing plant water extraction patterns across a topographic and hydrologic gradient at the ZF2 site near Manaus, Brazil. Here we expect drought conditions to be more extreme on the plateau where depth to water table is greater than in the valley. Second, we are testing plant water extraction patterns across a rainfall gradient for three sites in Panama. Here, we are also targeting species with varying drought tolerance/resistance levels to see if root water uptake depth helps explain sensitivity to drought. Plant water sourcing and rooting depth data will therefore improve the E3SM-FATES model and enhance the ability of this model to predict tropical forest response to climate change scenarios.

Title: **Increasing Impacts of Extreme Droughts on Vegetation Productivity under Climate Change**

Chonggang Xu[1*], Nate G. McDowell[2], Rosie A. Fisher[3, 4], Liang Wei[1, 5], Sanna Sevanto[1], Bradley O. Christoffersen[6], Ensheng Weng[7], Richard Middleton[1]

[1]Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM, USA; [2]Earth Systems Analysis & Modeling Division, Pacific Northwest National Laboratory, Richland, WA, USA; [3]Climate and Global Dynamics, National Center for Atmospheric Research, Boulder, CO, USA; [4]Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS), Toulouse, France; [5]Key Laboratory of Western China's Environmental Systems, College of Earth and Environmental Sciences, Lanzhou University, Lanzhou, Gansu, China;
[6]Department of Biology and School of Earth, Environmental, and Marine Sciences, The University of Texas Rio Grande Valley, Edinburg, TX, USA;
[7]Center for Climate Systems Research, Columbia University, and NASA Goddard Institute for Space Studies, New York, NY, USA

Contact: (cxu@lanl.gov)
Project Lead Principle Investigator (PI): Jeff Chambers, LBNL
BER Program: TES
Project: NGEE-Tropics
Project Website: https://ngee-tropics.lbl.gov/

Project Abstract: Terrestrial gross primary production (GPP) is the basis of food production and vegetation growth globally[1], and plays a critical role in regulating atmospheric CO_2 through its impact on ecosystem carbon balance. Even though higher CO_2 concentrations in future decades can increase GPP[2], low soil water availability, heat stress, and disturbances associated with droughts could reduce the benefits of such CO_2 fertilization. Here we analyzed outputs of 13 Earth System Models (ESMs) to show an increasingly stronger impact on GPP by extreme droughts than mild and moderate droughts over the 21st century. Due to a dramatic increase in the frequency of extreme droughts, the magnitude of globally-averaged reductions in GPP associated with extreme droughts was projected to be nearly tripled by the last quarter of this century (2075–2099) relative to that of the historical period (1850–1999) under both high and intermediate greenhouse gas emission scenarios. In contrast, the magnitude of GPP reduction associated with mild and moderate droughts was not projected to increase substantially. Our analysis indicates a high risk of extreme droughts to the global carbon cycle with atmospheric warming; however, this risk can be potentially mitigated by positive anomalies of GPP associated with favorable environmental conditions.

Title: Pantropical Patterns of Tropical Tree Damage and Death

Daniel Zuleta[1*], Gabriel Arellano[2], Stuart Davies [1]

[1] Forest Global Earth Observatory, Smithsonian Tropical Research Institute, Washington, DC;
[2] Ecology and Evolutionary Biology, University of Michigan, Ann Arbor, MI

Contact: (ZuletaD@si.edu)

Project Lead Principal Investigator (PI): Jeff Chambers, LBNL

BER Program: TES

Project: NGEE-Tropics

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

Project Abstract: Tropical forests are of utmost importance for the global carbon cycle and the world's biodiversity. Yet, our understanding of the likely response of tropical forests to the changing climatic conditions is very limited. This is partially attributed to the lack of a mechanistic inclusion of tree mortality in vegetation demographic models. Tree death not only has implications on the species demographic rates but on the biomass turnover times. Advancing in the understanding of the causes and consequences of tropical tree mortality is, therefore, a research priority to obtain more accurate predictions of the future of tropical forests and the carbon cycle-climate feedbacks. In order to expand the data available for developing and testing mechanistic models of tree mortality, we designed a protocol to perform annual tree damage and death assessments in large ForestGEO plots, as part of Phase I of the Next-Generation Ecosystems Experiments – Tropics (NGEE-Tropics) project. Here, we present results from 20 surveys, comprising over 100,000 (stem x time) observations made on 40,000 stems in seven sites across the tropics. The proportion of dead and damaged trees found standing, broken, and uprooted were significantly different among sites. These differences are likely related to patterns of forest disturbance and, thus, mortality drivers (e.g., winds, droughts) operating at regional and continental scales. Within forests, tree size and small-scale habitat differences emerged as important factors explaining the intra-plot variability in the probability of tree death and damage. The collateral damage of understory trees following crown loss and death of canopy trees was a conspicuous process across the tropics. In general, mortality linked to other variables such as loss of leaf area, leaf damage, lianas, wounds, or tumors was variable and site-specific. Long-term collection of tree death data will enable more robust annual climate-related tree mortality assessments, as well as the possibility to obtain more accurate estimates of woody residence times, and a better parametrization of stress-related damage associated with elevated mortality risks at the individual level.

Terrestrial Ecosystem Science

Argonne National Laboratory
TES Science Focus Area

Organic Matter Composition and Decomposability of Ice-Wedge Polygon Soils on the Coastal Plain of Northern Alaskan

Roser Matamala[1*], Julie Jastrow[1], Francisco Calderon[2], Chien-Lu Ping[3], and Umakant Mishra[1] [1] Argonne

National Laboratory, Lemont, IL
[2] Central Plains Resources Management Research, USDA. Akron, CO
[3] University of Alaska Fairbanks, Fairbanks, AK Contact: (matamala@anl.gov)

Project Lead Principal Investigator: Julie Jastrow BER Program: TES
Project: Argonne TES SFA (Soil Carbon Response to Environmental Change) Project Website: http://tessfa.evs.anl.gov/

The large stocks of soil organic carbon (SOC) in the northern permafrost region are sensitive to changes in global temperature and permafrost thawing. Furthermore, because the relative importance of SOC stabilization mechanisms operating in the permafrost region differ from those of other ecoregions, the composition and potential decomposability of soil organic matter (SOM) are key uncertainties in models projecting the amount of SOC that might be released from this region. In the search for indicators of decomposability that could be upscaled across the region, we have demonstrated that mid-infrared (MIR) spectroscopy is very sensitive to the degradation state of SOM and it is a good predictor of short-term carbon mineralization from tundra soils. In this study, we are expanding this work to explore the decomposability of a range of soil horizons at different depths in flat-, low-, and high-centered ice-wedge polygons formed on glaciomarine sediments (near Utqiaġvik, Alaska). The soils were incubated aerobically for over one year at two temperatures (15°C and 5°C), and CO_2 production was measured every 12 h for the first 2-3 months and every 3 weeks thereafter. Results to date indicate that excellent partial least square regression (PLSR) models of cumulative CO_2 production at 15°C expressed on a soil mass basis can be derived from the MIR spectra of bulk soil for intervals of 1 to 12 months incubation times. The PLSR models could also predict short-term CO_2 production on a SOC basis, and predictions were better when low carbon (<10%) and high carbon (>10%) soils were predicted separately. This suggests that the spectral relationship of MIR with CO_2 production in incubation studies reflects both the quantitative and qualitative properties of SOC. This experiment confirms the power of soil MIR spectra to predict C mineralization from Arctic soils. 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.

Digital Tools for Advanced Analysis and Comparison of Irregular Carbon Distributions in Cryoturbated Soil Profiles

Julie Jastrow[1*], Nicolas Jelinski[2], Roser Matamala[1], Chien-Lu Ping[3], and Umakant Mishra[1] [1] Argonne National Laboratory, Lemont, IL
[2] University of Minnesota-Twin Cities, St. Paul, MN
[3] University of Alaska Fairbanks, Fairbanks, AK Contact: (jdjastrow@anl.gov)

Project Lead Principal Investigator: Julie Jastrow BER Program: TES
Project: Argonne TES SFA (Soil Carbon Response to Environmental Change) Project Website: http://tessfa.evs.anl.gov/

Cryoturbated permafrost-affected soils are often characterized by patterned ground on the surface (e.g., frost boils, stripes, or ice-wedge polygons) and by irregular and broken horizons belowground. Consequently, these soils are not well represented by typical one-dimensional soil profile descriptions that assume laterally continuous horizons for determining the distribution of soil organic carbon stocks and other soil constituents. Two-dimensional representations of soil profiles allow for more accurate spatial and vertical characterization by accounting for the area of each soil horizon or layer within each incremental horizontal or vertical slice of interest within the profile. This approach enables quantitation of soil constituents for the entire cycle of a patterned-ground pedon (generally about 1-2 m in size) or super-pedon, as typified by ice-wedge polygons (often 5-30 m across). We have generated a workflow using open-source geographic information system software (QGIS) and the R programming language/environment to digitize, scale, and rasterize two-dimensional drawings of soil profiles. Following rasterization, raster attribute tables (RATs) are built for each morphologic unit within the profile (referred to as "soil morphologic units" or SMUs). RATs can include field characterization and laboratory data for each SMU or SMU component. Analogous to soil mapping concepts, the representation of various component units within delineated SMUs is also possible. This digitization and rasterization workflow enables the quantitative analysis of two-dimensional profiles as well as their synthesis with standard one-dimensional soil profile descriptions (or observations from soil cores) via tools such as Algorithms for Quantitative Pedology (AQP; Beaudette et al., 2013, Computers & Geosciences 52:258-268). By coupling the rasterized profile images with R scripts, quantitation of carbon and nitrogen stocks or other measured soil constituents can now be easily and rapidly determined for any depth or horizontal increment and compared among multiple pedons or super-pedons. Importantly, these tools allow for improved harmonization of disparate data sources and data formats without information loss and, thereby, will enable more accurate geospatial analyses and mapping efforts, which are needed to benchmark landscape, regional, and Earth system model predictions for high latitude soils.

Ensemble Machine Learning Improves Predicted Spatial Heterogeneity of Surface Soil Organic Carbon Stocks in the Data-Limited Northern Circumpolar Permafrost Region

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

[1] Argonne National Laboratory, Lemont, IL Contact: (umishra@anl.gov)

Project Lead Principal Investigator: Julie Jastrow BER Program: TES
Project: Argonne TES SFA (Soil Carbon Response to Environmental Change) Project Website: http://tessfa.evs.anl.gov

Various approaches of differing mathematical complexities are being applied for spatial prediction of soil organic carbon (SOC) stocks. Regression kriging is a widely used hybrid approach for spatial prediction that combines correlation between soil properties and environmental factors with spatial autocorrelation among soil observations. In this study, we compared four machine learning approaches (gradient boosting machine [GBM], multi-narrative adaptive regression spline [MARS], random forest [RF], and support vector machine [SVM]) with regression kriging to predict the spatial heterogeneity of surface (0-30 cm) SOC stocks at 250-m spatial resolution across the northern circumpolar permafrost region. We combined 1660 soil profile observations (calibration datasets) with georeferenced datasets of environmental factors (climate, topography, land cover, bedrock geology, and soil types) to predict the spatial heterogeneity of surface SOC stocks. We evaluated the prediction accuracy at 714 randomly selected sites (validation datasets) across the study area. We found that different techniques inferred different numbers of environmental factors and their relative importance for prediction of SOC stocks. Among all machine learning approaches, temperature, latitude, land cover types, slope, and elevation had higher impacts on the predicted spatial heterogeneity of surface SOC stocks. In addition to these environmental factors, soil types were also important predictors of surface SOC stocks in the regression kriging approach. Regression kriging produced lower prediction errors in comparison to MARS and SVM, and comparable prediction accuracy to GBM and RF. However, the ensemble median prediction of SOC stocks obtained from all four machine learning techniques produced the best prediction accuracy. The uncertainty in surface SOC stocks predicted by this ensemble machine learning approach was less than 20% in about half of the study area. Areas with high uncertainty (>50% uncertainty) in predicted SOC stocks were observed in small patches in southern Alaska and Iceland, and in larger areas of the southern and western Russian permafrost region. Although the use of different approaches in spatial prediction of soil properties will depend on the availability of soil and environmental datasets and computational resources, we conclude that the ensemble median prediction obtained from multiple machine learning approaches provides greater spatial details and produces the highest prediction accuracy. Thus, an ensemble prediction approach can be a better choice than any single prediction technique for predicting the spatial heterogeneity of SOC stocks.

Terrestrial Ecosystem Science

Lawrence Berkeley National Laboratory
TES Science Focus Area

The Berkeley Lab Terrestrial Ecosystem Science SFA on Belowground Biogeochemistry: Five years of deep soil warming

Margaret S. Torn[1*], Eoin Brodie[1], Peter Nico[1], Bill J. Riley[1], Cristina Castanha[1], Rachel C. Porras[1], Jennifer L. Soong[1], Ricardo E. Alves[1], Zhou Lyu[1].

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

(mstorn@lbl.gov)

BER Program: TES
Project: Berkeley Lab TES SFA on Belowground Biogeochemistry
Project Website: https://eesa.lbl.gov/projects/terrestrial-ecosystem-science/

In the Berkeley Lab Terrestrial Ecosystem Science SFA, we conduct basic research on the role of soils in terrestrial biogeochemistry and the Earth system. Our goals are to improve process-level understanding of ecosystem-climate interactions and to develop next-generation predictive capacity suitable for Earth system models. Current SFA research is centered around a set of field, laboratory, and model experiments to characterize how biotic and abiotic processes influence soil carbon cycling, and how they may shape ecosystem responses to a warming climate. We are conducting a field experiment in a well-drained coniferous forest in which we are warming the whole soil profile (+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. We are using experimental data from the deep soil warming, incubations, and other studies to guide model development in a reactive transport framework (BeTR; Tang et al. 2013), and integrating this into the DOE E3SM land model (ELM). This poster will present biogeochemistry results from the Blodgett Forest whole soil warming experiment over its first five years. Research on microbiology, mineralogy, and modeling are described in abstracts by Alves, Nico, and Lyu respectively.

During the first two years of the experiment, warming increased total CO_2 respiration by 35% (Hicks Pries et al. 2016). After five years of warming (spanning both wet and drought years), soil respiration continued to average 30% higher compared to the control plots with no trend in the effect size. Decomposition, as measured by soil CO_2 production, was significantly higher in the subsurface (>20 cm depth). Moreover, by year five, we documented a significant decrease in soil carbon stocks due to heating, particularly below 50 cm depth.

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

Applying the ELM Microbial-explicit Soil Biogeochemical Model to Analyze Carbon Responses to Whole Soil Profile Warming

Zhou Lyu[1]*, William Riley[1], Jinyun Tang[1], Rose Abramoff[2], Jennifer Soong[1], Cristina Castanha[1], and Margaret S. Torn[1]

[1] Lawrence Berkeley National Laboratory, Berkeley, CA
[2] Le Laboratoire des Sciences du Climat et de l'Environnement, Paris, France

BER Program: TES
Project: Berkeley Lab Terrestrial Ecosystem Science SFA
Project Website: https://tes.lbl.gov/

Project Abstract: Soil organic carbon is the largest actively cycling component of global terrestrial carbon and is vulnerable to climate changes, such as warming. Therefore, it is desirable to accurately assess how this large carbon pool responds to increasing temperature. Here we use a comprehensive microbe and mineral-surface explicit soil biogeochemical model integrated in the E3SM land model (ELM) to simulate soil carbon dynamics in a warming environment. To calibrate and evaluate the model, we apply field observations from one of the few on-going whole soil profile warming experiments, the LBNL TES SFA Warming Experiment at the Blodgett Experiment Forest in the Sierra Nevada Mountains, California. Three plots at this temperate conifer forest have been warmed by 4℃ for over 4 years to 1m depth, and soil fluxes and stocks are been monitored and compared to adjacent control plots. We conduct both ambient and heated simulations using CRU climate forcing corrected with site weather station data. Observed depth-resolved soil temperature and soil moisture are imposed for the heated simulation. We will present modeling results in comparison to the field observation results at this warming site from 2014 to 2018, for both control and heated plots. The model accurately represents observed soil surface CO_2 fluxes, soil carbon stocks and microbial biomass. Heated simulations capture the observed increase in soil CO_2 fluxes and decrease in carbon stocks compared to controls. Soil respiration from the heated simulations are over 20% higher than the control simulations each year, especially for wet winters and springs. This pattern indicates that seasonal variation of soil moisture and temperature affect soil carbon dynamics and the magnitude of the warming effect. Comparing the inter-annual soil flux responses, we find slightly higher soil surface fluxes at the beginning of the warming period. During this period, the soil microbial community may have been reorganizing, pointing to a possibility of an acclimation trend in the longer term. Finally, we find that heating caused soil carbon losses in the sub-soil, emphasizing the importance of carbon stored in deeper soils under warming climate.

Stabilization of Mineral Associate Simple Organic Molecules Under Varying Temperature and Moisture Conditions-- LBNL TES SFA

Rachel Porras,[1] Peter Nico[1]*, Cristina Castanha[1], Jennifer Soong[1], Eoin Brodie[1], Bill Riley[1], Margaret S. Torn[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA

(Peter Nico psnico@lbl.gov)

BER Program: TES
Project: Terrestrial Ecosystem Science Focus Area
Project Website: https://eesa.lbl.gov/projects/terrestrial-ecosystem-science/

Project Abstract:Soils represent an important reservoir of organic carbon. However, the accessibility of soil C and, in particular mineral-associated organic C, to microbial decomposer communities and its response to changing temperature and moisture regimes remains uncertain. To gain insight into the decomposability of mineral-associated organic C and the sensitivity of mineral associated C to environmental perturbations, we conducted a series of incubations using different types of synthetic mineral organic associations (MOAs), incubating those MOAs in soils from different depths (10-20 and 80-90 cm), and varying temperature and moisture conditions in the incubations. The two types of MOA included 13C labeled glucose or 13C labeled glycine associated with one of two different Fe (hydr)oxides. The soils are moderately acidic (pH ~6.5) sandy, mixed, mesic Ultic Haploxeralfs from a coniferous forest. The soils containing the 13C labeled MOAs were incubated at two temperatures: 25 deg. C and 30 deg. C. Additionally, the glucose containing MOA was also incubated at two different moisture levels: 20% and 30% VMC. CO_2 concentration and d13C measured for synthetic MOA treated soils were compared to a natural abundance (no added 13C label or mineral) control and a non-mineral associated 13C glucose control. Perhaps not surprisingly, increases in temperature and moisture induced significant changes in decomposition of native SOC across all treatments and in both depths. However, sorption of either organic molecule to reactive mineral surfaces dramatically decreases decomposability under all experimental conditions relative to the free substrate. Additional suggested conclusions include that decomposition of MOA bound glucose is more sensitive to temperature and moisture perturbations than non-mineral associated glucose. In addition, it appears that overall temperature and moisture effects on native SOC were roughly additive whereas for the mineral bound organics the impacts were clearly not additive. It is hypothesized that this result can be explained by assuming that increases in either temperature or moisture have the impact in increasing the release of a finite pool of weakly organic matter. Since both variables act on the same pool, their impact is limited by the total quantity of weakly bound organic matter and therefore the impacts are not fully additive. If correct, the hypothesis can inform the numerical modeling of MOA dynamics in as much as it implies the need to represent a distribution of association strength with the fraction of organic associated in order to accurately capture the response of soil carbon stocks to temperature and moisture variation.

LBNL TES SFA—Kinetic Properties and Temperature Sensitivity of Microbial Exoenzymes Through the Soil Profile.

Ricardo J. E. Alves[1]*, Ileana Callejas[1,2], Ulas Karaoz[1], Margaret S. Torn[1,3], Eoin L. Brodie[1,3]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]University of California, Los Angeles, CA;
[3]University of California, Berkeley, CA.

(rjealves@lbl.gov)

BER Program: TES
Project: Berkeley Lab Terrestrial Ecosystem Science SFA
Project Website: https://tes.lbl.gov/

Project Abstract: Current knowledge of the mechanisms and responses of soil organic matter (SOM) decomposition to warming remains incomplete, and is mostly limited to surface soils. However, over 50% of global soil carbon is contained in sub-soils, characterized by different physicochemical conditions, nutrient inputs, and SOM chemistry. Such factors select for microbiomes with distinct functional traits that may constrain SOM decomposition responses to warming. In the LBNL TES SFA, we are investigating microbial traits and feedbacks to warming through the soil profile using continuous field-based experiments and laboratory manipulations. Soil exoenzymes represent fundamental traits of microbes, and mediate the rate-limiting step in SOM decomposition by liberating the assimilable products required by microbes and plants. We hypothesized that microbial exoenzyme properties are optimized to the substrate availability and temperature regimes of their soil horizon, and integrate broader trait spaces that reflect the life strategies and ecophysiology of microbes at depth. Here, we determined the Michaelis-Menten kinetics and temperature sensitivity of three ubiquitous enzymes involved in carbon, nitrogen and phosphorus acquisition across a broad range of soil depths and temperatures, in soils from our field site in a mixed coniferous forest underlain by alfisols at Blodgett, CA. We observed that maximal reaction rates (Vmax) decreased with depth, whereas their affinities (Km) increased, indicating adaptation to lower substrate availability. Enzyme Vmax, affinity and catalytic efficiency increased consistently with temperature, indicating higher SOM depolymerization potential with warming, although their temperature sensitivity (Q10) did not change substantially with depth. Also, the N-acquiring enzyme had much lower affinity and catalytic efficiency, suggesting that nitrogen is relatively less limiting to microbes than other nutrients. Moreover, we are investigating relationships and trade-offs between measured enzyme properties and genetic trait distribution/expression, and SOM chemistry, inferred from meta-omics data from the ongoing whole-soil profile warming experiment at Blodgett. This information will be used to test and validate the representation of depth-dependent microbial traits in biogeochemical models.

Terrestrial Ecosystem Science

Oak Ridge National Laboratory
TES Science Focus Area

Title: **Ecosystem Warming Accelerates Peatland Carbon Loss: Findings from the First Three Years of SPRUCE**

Natalie A. Griffiths,[1]* Paul J. Hanson,[1] Colleen M. Iversen,[1] Richard J. Norby,[1] Stephen D. Sebestyen,[2] Jana R. Phillips, [1]Jeffrey P. Chanton,[3] Randall K. Kolka,[2] Avni Malhotra,[4] Keith C. Oleheiser,[1] Jeffrey M. Warren,[1] Xiaoying Shi,[1] Xiaojuan Yang,[1] Jiafu Mao,[1] Daniel M. Ricciuto[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]USDA Forest Service, Northern Research Station, Grand Rapids, MN;
[3]Florida State University, Tallahassee, FL;
[4]Stanford University, Stanford, CA

Contact: (griffithsna@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://mnspruce.ornl.gov/

Project Abstract: One-third of the Earth's terrestrial C is found in peatland ecosystems, and the majority of this C has accumulated belowground over millennia. Because of the disproportionate importance of peatlands to the global terrestrial C budget, it is critical to understand how peatland C responds to warming and elevated atmospheric CO_2. The Spruce and Peatland Responses Under Changing Environments (SPRUCE) project is evaluating the effects of warming and elevated CO_2 on an ombrotrophic bog in northern Minnesota using a novel ecosystem-scale experiment: 10 enclosures (12-m diameter, 8-m tall) that span a range of warming conditions (+0 ºC, +2.25 ºC, +4.5 ºC, +6.75 ºC, +9 ºC) at ambient CO_2, and replicated at elevated CO_2 (+500 ppm). The experiment began in August 2015 and is planned to run for a decade. Here, we examined the response of peatland net C flux to warming and elevated CO_2 during the first three full years of the experiment (2016-2018). Net C flux was calculated from measurements of tree and shrub net primary production (NPP; above and belowground), *Sphagnum* NPP, CO_2 and CH_4 efflux from the bog surface, and total organic carbon (TOC) and dissolved inorganic carbon (DIC) efflux in lateral outflow. Overall, there was a strong linear response of C flux to warming with a net C loss of 34.5 g C m^{-2} y^{-1} $°C^{-1}$. Peatland C loss was primarily driven by decreased *Sphagnum* NPP and increased losses of CO_2 and CH_4. *Sphagnum* was the predominant contributor to aboveground NPP in this peatland, and production decreased drastically in 2017 and 2018 with warming due to reduced growth and loss of ground cover. Both CO_2 and CH_4 losses increased with warming in all years, and while the magnitude of CO_2 efflux was much larger than that of CH_4, the response of CH_4 efflux to warming was stronger. In summary, we found that the bog switched from a net C sink under ambient conditions to a net C source with warming. Evaluation of peatland net C flux will continue for the duration of SPRUCE to examine if: 1) the peatland continues to be a source of C under warming, 2) the response continues to be linear, and 3) effects of elevated CO_2 begin to emerge.

Title: **What is the Effect of Climate Change on Belowground Resource Acquisition Strategies in a Boreal Peatland?**

Camille Defrenne,[1]* Joanne Childs,[1] Paul J. Hanson,[1] Colleen M. Iversen[1]

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

Contact: (defrennece@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://mnspruce.ornl.gov/

Project Abstract: Belowground biotic interactions govern the world's largest terrestrial carbon sink: peatlands. Below the peat surface, the finest, most absorptive plant roots interact with mycorrhizal fungi by supplying them with photosynthates in exchange for soil nutrients. Without their fungal symbionts that use carbon and nutrient-degrading enzymes, plants would struggle to acquire enough resources from the saturated organic peat. Yet, much remains to be done to understand the response of this symbiotic interaction to climate change and its impact on peatland carbon cycling. We are examining the functional traits of fine roots and mycorrhizal fungi in the Spruce and Peatland Responses Under Changing Environments (SPRUCE) experiment in Northern Minnesota to detect potential shifts in belowground resource acquisition strategies with warming and elevated CO_2. We used ingrowth cores to quantify the variation in specific root length, root diameter, tissue density, nitrogen concentration, and in ectomycorrhizal (colonization rate, exploration type and enzymatic activity) and ericoid mycorrhizal (colonization rate) functional traits. After three years of warming, we show that a change in resource acquisition strategy of *Larix laricina* and *Picea mariana* occurs when the warming level reaches +4.5 °C. At this warming level, the degree of colonization of fine roots by ectomycorrhizal fungi is relatively high compared to the +0 and + 9 °C treatments, while specific root length slightly increased. This suggests that, with warming, tree fine roots tend to adopt an intensive resource acquisition strategy in which they rely more on mycorrhizal fungi to get soil resources. We are verifying this result with cores collected after four years of warming. We are also analyzing time series of minirhizotron images collected using new, high-resolution automated minirhizotrons. We will discuss preliminary results focused on the abundance and dynamics of fine roots, ectomycorrhizal root tips, and fungal mycelial system.

Title: Plant Physiological Response to Whole Ecosystem Warming and Elevated CO_2 – Can Bog Plants Be Water Stressed?

Jennifer Peters,[1]* Jeffrey M. Warren[1]

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

Contact: (petersjm@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory)
Project Website: https://mnspruce.ornl.gov/

Project Abstract: The last few decades of warming studies and elevated CO_2 experiments have taught us how terrestrial plants react to different environmental conditions, ever informing model predictions of a changing world. At the southern edge of the boreal forest we use large open-top enclosures to expose a forested bog to whole ecosystem warming and elevated CO_2, taking forest manipulation experiments to the next level to investigate the intersection of the temperature and CO_2 responses. Our goal is to answer the questions: "What is the interaction between these temperature and CO_2 responses in a mature natural forest?" and "How do the paradigms we know and understand about plant physiology under climate change conditions hold up in a wetland?"

We know that: 1) warming is likely to stimulate decomposition, potentially increasing nutrient availability for plants, and could extend the growing season as plants green-up earlier in the spring; 2) elevated CO_2 should make photosynthesis more efficient; and 3) reliable water availability from the bog should alleviate water stress, which has been exhibited by other terrestrial systems that experience warming. Perhaps climate change conditions will unleash the productivity potential of these cold tolerant plants?

After three years of experimental treatments at the Spruce and Peatland Responses Under Changing Environments (SPRUCE) site, we find elevated CO_2 concentrations stimulates photosynthesis and growth, but ecosystem warming challenges plants with increased water stress and higher risk of spring freeze damage. We have witnessed crown damage, branch tip dieback and mortality in the dominant tree and shrub species and, in investigating it, have discovered that even bog plants can be water stressed. While the bog plant community have only a small number of species, we have found wide diversity in hydraulic strategies, from conservative to risky, resulting in divergent carbon dynamics among the species.

Title: Understanding the Relative Importance of Nitrogen Versus Phosphorus Cycling in an Undisturbed Ombrotrophic Bog: Insight into Ecosystem Response to SPRUCE Manipulations

Verity G. Salmon[1,*], Randy Kolka,[2] Colleen M. Iversen,[1] Natalie Griffiths,[1] Steve Sebestyen,[3] Richard J. Norby,[1] Xiaojuan Yang,[1] Deanne J. Brice,[1] Joanne Childs,[1] Holly M. Vander Stel,[3] Avni Malhotra,[4] Jake Graham,[5] Jana Phillips,[1] Paul J. Hanson[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Northern Research Station, USDA Forest Service, Grand Rapids, MN;
[3]Kellogg Biological Station, Michigan State University, Hickory Corners, MI;
[4]Stanford University, Stanford, CA;
[5] Department of Geosciences, Boise State University, Boise, ID

Contact: (salmonvg@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://mnspruce.ornl.gov/

Project Abstract: Peatlands store one third of global soil C and this large pool of C has accumulated due to productivity outpacing decomposition. In northern peatlands, however, rapid warming threatens to accelerate peat decomposition, potentially causing a net release of C to the atmosphere. The future C balance of peatland systems will likely be mediated in part by the availability of nutrients, especially in ombrotrophic bogs where plant productivity hinges on deposition of nitrogen (N) and phosphorus (P) due to slow decomposition and nutrient recycling under cold, wet, and acidic conditions. To better understand the relative importance of these two nutrients in an ombrotrophic bog, we combined field observations and literature data to build comprehensive N and P budgets for the S1 bog at Marcell Experimental Forest. The S1 bog is a well-studied ecosystem and the site of the Spruce and Peatlands Under Changing Environments (SPRUCE) experiment where warming and elevated CO_2 treatments are applied in a regression-based design. While peatlands are known to be strongly nutrient-limited, our results show that both N and P are lost from the S1 bog ecosystem prior to treatment application. N losses are over four times higher than P losses (6.05 gN/ha/yr versus 1.27 gP/ha/yr), but both N and P losses are driven primarily by lateral outflow from the bog surface. Annual net primary productivity (NPP) of plants requires 101.80 ± 165.25 gN/ha/yr (N_{req}) and 8.28 ± 16.80 gP/ha/yr (P_{req}). NPP of *Sphagnum* moss is the strongest driver of both N_{req} and P_{req} at the ecosystem scale, making up 46% and 42% of the total nutrient requirements. N_{req} and P_{req} are met predominantly through recycling of N and P, with new inputs meeting only 5% and 0. 8% of the demand for N and P respectively. Together, the smaller P losses and smaller proportion of P_{req} met by inputs indicate that P cycle is more tightly constrained than the N cycle at the S1 bog. Low P availability may be particularly limiting for growth of the trees (*Picea mariana* and *Larix laricina*) since N_{req}:P_{req} is lower for trees than *Sphagnum* or understory plants (9 vs 13 & 15). Our results show that the response of the S1 bog to SPRUCE manipulations will likely depend on internal cycling of N versus P through plants and soils and accurate modeling of nutrient dynamics will be crucial to projecting the future C balance of the ombrotrophic bogs.

Title: Warming Increases Plant-Available Nitrogen and Phosphorus in the SPRUCE Bog

Colleen M. Iversen,[1]* John Latimer,[1] Deanne J. Brice,[1] Joanne Childs,[1] Holly M. Vander Stel,[2] Natalie Griffiths,[1] Avni Malhotra,[3] Richard J. Norby,[1] Keith Olehieser,[1] Steve Sebestyen,[4] Verity G. Salmon,[1] Jana Phillips,[1] Paul J. Hanson[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Kellogg Biological Station, Michigan State University, Hickory Corners, MI;
[3]Stanford University, Stanford, CA;
[4]Northern Research Station, USDA Forest Service, Grand Rapids, MN

Contact: (iversencm@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://mnspruce.ornl.gov/

Project Abstract: 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. We used ion-exchange resin capsules to monitor monthly *in situ* changes in plant-available nutrients (i.e., NH_4-N, NO_3-N, and PO_4-P) throughout the peat profile across hummock-hollow microtopography in the experimental plots. NH_4-N was by far the most available N source, with NO_3-N making up a negligible fraction; PO_4-P availability was intermediate. Warming, combined with a longer frost-free period, increased the availability of NH_4-N and PO_4-P in the warmest treatment plots between two and twenty-fold. The increase in nutrients was much greater in deeper peat, beneath the rooting zone. There is thus far no clear 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-N, NO_3-N, or PO_4-P concentrations across the warmed plots.
Taken together, these lines of evidence indicate that warming has increased the mineralization of organic peat, leading to increased mineral nutrient availability. In turn, the 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 were detectable in *Sphagnum* mosses as well as vascular plant tissues; however, in recent years we observed a drastic increase in available NH_4-N and PO_4-P in shallow peat in the warmest plots where *Sphagnum* cover was decimated. The relative balance of peat accumulation will be affected by the interplay between vegetation dynamics and changing environmental conditions, mediated by nutrient and water availability.

Title: An Investigation of the Role of Methoxylated Aromatic Compounds in Methanogenesis from Peat and an Update on Ongoing SPRUCE Metagenomic Analyses

Eric R. Johnston,[1] Rachel N. Andrews,[1,2] Paul J. Hanson,3 and Christopher W. Schadt[1]*

[1]Biosciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Roane State Community College, Harriman, TN
[3]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;

Contact: (schadtcw@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: http://mnspruce.ornl.gov

Project Abstract: Boreal peatlands are simultaneously important ecosystems for terrestrial carbon storage as well as large sources of the greenhouse gas methane. Methanogenic Archaea are thought to primarily use acetoclastic (acetate), hydrogenotrophic (carbon dioxide and hydrogen) or methylotrophic (C-1 compounds) pathways and substrates to produce methane. Recently, an organism using Methoxylated Aromatic Compounds (MACs) to produce methane was characterized from coal bed systems, however the prevalence, ecology and detailed mechanisms of these organisms and pathways remain unknown. As MACs are common in peat, we conducted laboratory microcosm experiments using peat from the SPRUCE site and six different methoxylated aromatic compounds to peat from various depths in the peat profile and incubated anaerobically for ~100 days. Gas headspace was monitored for CH_4 and CO_2 over time and final samples were harvested for microbial analysis using 16S rRNA gene sequencing. Experiments to date show a high heterogeneity in gas production response to MAC amendment across peat cores and depths within core profiles. Rates of methanogenesis were generally slow, but increased over the course of incubation period (up to 0.94 ug C-CH_4 / g peat per day vs. 0.26 in controls), as did the CH_4:CO_2 ratio of headspace gases (up to 12.82 vs. 0.96 in controls), and were highest with 2-methoxyphenol, 1,3,5-trimethoxybenzene, and 3,4,5-trimethoxybenzyl alcohol additions. Several MAC incubations produced significantly more methane than no-substrate controls as well as methanol used as a comparative known methylotrophic substrate. Together results to date suggest that MAC utilizers are present in peatland systems but may be in low abundance, and that high concentrations of certain methoxylated compounds may have toxic effects on some microbes. DNA analysis of microbial communities are ongoing and follow up experiments are being designed with ^{13}C-labeled substrates to better distinguish MAC methanogenesis from other potential pathways. When complete these investigations should provide valuable insights the prevalence and mechanisms for MAC based methanogenesis in peatland ecosystems. In addition to these MAC experiments, an update on new metagenomic analyses of microbial community changes during the SPRUCE experimental treatments will be presented resulting from data just coming in via a collaboration with the Joint Genome Institute.

Title: Modeling the Hydrology and Physiology of *Sphagnum* Moss in a Northern Temperate Bog

Xiaoying Shi,[1]* Daniel M. Ricciuto,[1] Peter E. Thornton,[1] Xiaofeng Xu, [2]Fengming Yuan,[1] Richard J. Norby, [1]Anthony P. Walker, [1]Jeffrey Warren,[1] Jiafu Mao,[1] Paul J. Hanson,[1] David Weston,[3] Lin Meng,[4] Natalie A. Griffiths[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]Biosciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN
[4]Department of Geological and Atmospheric Sciences, Iowa State University, Ames, IA

Contact: (shix@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://mnspruce.ornl.gov/

Project Abstract: Mosses need to be incorporated into Earth system models to better simulate peatland functional dynamics under changing environments. *Sphagnum* mosses are strong determinants of nutrient, carbon and water cycling in peatland ecosystems. However, most land surface models do not include *Sphagnum* or other mosses as represented plant functional types (PFTs), thereby limiting predictive assessment of peatland responses to environmental change. In this study, we introduce a moss PFT into the land model component (ELM) of the Energy Exascale Earth System Model (E3SM), by developing water content dynamics and non-vascular photosynthetic processes for moss. The model was parameterized and independently evaluated against observations from an ombrotrophic forested bog as part of the Spruce and Peatland Responses Under Changing Environments (SPRUCE) project. Inclusion of a *Sphagnum* PFT with some *Sphagnum*-specific processes in ELM allows it to capture the observed seasonal dynamics of *Sphagnum* gross primary production (GPP), albeit with an underestimate of peak GPP. The model simulated a reasonable annual net primary production (NPP) for moss but with less interannual variation than observed and reproduced aboveground biomass for tree PFTs and stem biomass for shrubs. Different species showed highly variable warming responses under both ambient and elevated atmospheric CO_2 concentrations; and elevated CO_2 altered the warming response direction for the peatland ecosystem. Microtopography is critical: *Sphagnum* mosses on hummocks and hollows were simulated to show opposite warming responses (NPP decreasing with warming on hummocks, but increasing in hollows), and hummock *Sphagnum* was modeled to have strong dependence on water table height. Inclusion of this new moss PFT in global ELM simulations may provide a useful foundation for the investigation of northern peatland carbon exchange, enhancing the predictive capacity of carbon dynamics across the regional and global scales.

Title: Evaluating ELM-SPRUCE Using Carbon Isotope Measurements

Xiaojuan Yang,[1]* Dan Ricciuto,[1] Paul Hanson,[1] Colleen Iversen,[1] Karis McFarlane[2]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Lab, Oak Ridge, TN;
[2]Atmospheric, Earth, and Energy Division, Lawrence Livermore National Lab, Livermore, CA

Contact: (yangx2@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: http://mnspruce.ornl.gov

Project Abstract: Peatland ecosystems store about one third of global soil carbon(C) and play an important role in the global C cycle. Yet, the representation of peatland responses to global changes in Earth System Models (ESMs) remains a challenge due to the complex interactions between climate, hydrology, plant physiology, allocation, turnover and soil biogeochemistry. The development of Earth Land Model (ELM)-SPRUCE allows us to explore these complex interactions by taking advantage of the comprehensive measurements at SPRUCE sites. ELM-SPRUCE has been evaluated and improved by using field observed carbon, nitrogen, and phosphorus pools and fluxes. Measurements of carbon isotopes (^{13}C and ^{14}C) provide additional opportunity for model evaluation. The goal of this study is to evaluate the performance of ELM-SPRUCE against carbon isotope measurements at the SPRUCE site and identify the areas for further model improvement. We first evaluate model simulated soil $\Delta^{14}C$ vertical profile against baseline measurements. Our results suggest that the model captures the shape of the measured $\Delta^{14}C$ vertical profile very well, except for the surface layer where model simulated $\Delta^{14}C$ is more negative than measurements. This could be due to the inaccurate representation of vertical movement of soil organic matter. We also take advantage of the unique isotope signal of the added CO_2 in elevated CO_2 plots to evaluate the representation of allocation and turnover in the model. Preliminary results show that the model is able to capture the observed $\Delta^{14}C$ of vegetation in elevated CO2 plots. Detailed evaluation of tissue turnover is underway.

Title: Modification and Evaluation of ELM Seasonal Deciduous Phenology Against the SPRUCE Observations

Jiafu Mao,[1]* Lin Meng, [2]Daniel M. Ricciuto,[1] Xiaoying Shi,[1] Paul J. Hanson[1]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Department of Geological and Atmospheric Sciences, Iowa State University, Ames, IA

Contact: (maoj@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://tes-sfa.ornl.gov; https://mnspruce.ornl.gov

Project Abstract: Phenology transitions determine the timing of changes in land surface properties (e.g., albedo and roughness) and exchanges of biosphere-atmosphere materials (e.g., carbon, energy, and water). However, current phenological processes for seasonal deciduous plant types in the land component of the US Department of Energy's (DOE) Energy Exascale Earth System Model (ELM of E3SM) are based solely on growing-degree-day model (onset) and a fixed daylength threshold (offset). Thus, they are limited in characterizing the long-term phenological responses under changing environmental conditions, causing large uncertainties in the prediction of land-atmosphere interaction. We introduced new phenology onset and offset models to seasonal-deciduous forest and shrub, respectively, in which the timing of plant development depends on various environmental cues (forcing and chilling processes for onset, and daylength and air temperature for offset). The modified models were calibrated and evaluated using the unique phenology observations (i.e., the PhenoCam) in the Spruce and Peatland Responses Under Climatic and Environmental Change experiment (SPRUCE) in northern Minnesota. Compared to the default phenology algorithms, the revised models were found to better represent the deciduous phenology for both deciduous forest and shrub, in terms of the timing magnitudes and phenological responses to different warming treatments, especially for autumn offset. Moreover, the updated ELM with revised phenology schemes generally produced higher land fluxes (e.g., GPP and evapotranspiration) than those simulated by the default ELM because of the lengthened growing season induced mainly by the later offset. This modeling effort also demonstrates the potential to enhance the E3SM representation of land-atmosphere feedbacks at broader spatial scales, especially under anticipated warming conditions when chilling might limit the rate of spring onset advance and offset may continue to delay.

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

Jeffrey M. Warren,[1]* Hassina Bilheux,[2] Keita DeCarlo,[3] Edmund Perfect,[4] Katie Marcacci,[4] J Aaron Hogan,[5]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Neutron Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN;
[3]Princeton University, Princeton, NJ;
[4]University of Tennessee, Knoxville, TN;
[5]Florida International University, Miami, FL

Contact: (warrenjm@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://tes-sfa.ornl.gov

Project Abstract: Assessment of root function *in situ* is extremely difficult, but advances in imaging technology are allowing unprecedented insight into root dynamics. Neutron imaging is highly sensitive to hydrogen ions, thus biological material and water are readily visible, which allows for *in situ* assessment of root structure, root growth, root water uptake, and internal root water transport. Results with various woody plants, maize, and switchgrass indicate significant variability in water dynamics across the soil-rhizosphere-root pathway, including root water uptake and hydraulic redistribution, hysteresis in water release curves and soil wettability. Measured root water extraction rates by cottonwood ranged from 0.003 to 0.02 g cm^{-2} h^{-1}, with lower rates for larger roots. Across species, root rhizosphere development increases with root size, stabilizing as roots reach ~2 mm in diameter. Analysis required development of a novel “RootProcessing” image analysis software to identify and segment roots, and analyze root, rhizosphere and soil water dynamics. Neutron radiography has also indicated significant root and mycorrhizal impacts to the soil hydraulic parameters, including hydraulic conductivity and residual water content. Results are important for testing and improving models of root water uptake and its linkages to root traits. Other key root processes that models are sensitive to include dynamics of root carbon allocation, relationships between roots and mycorrhizal fungi, root nutrient uptake, and root respiration and acclimation to temperature. Here, we leverage neutron imaging techniques to assess in situ root water dynamics, and hyphal exclusion or root exclusion chambers to asses in situ respiration dynamics in response to environmental changes.

Title: Understanding Taxonomic, Environmental, and Mycorrhizal Influences on Fine-Root Trait Variation Using the Global Fine-Root Ecology Database (FRED)

Yao Liu, [1]* M. Luke McCormack,[2] Kiona Ogle,[3] Anthony P. Walker,[1] Colleen M. Iversen[1]

[1]Environmental Science Division [and] Climate Change Science Institute and, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Center for Tree Science, The Morton Arboretum, Lisle, IL;
[3]School of Informatics, Computing, and Cyber Systems, Northern Arizona University, Flagstaff, AZ,

Contact: (liuy6@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://tes-sfa.ornl.gov

Project Abstract: Fine roots (< 2 mm in diameter) perform essential plant functions such as nutrient and water acquisition. Linking plants and the soil, they also play a central role in belowground carbon cycling and storage. However, unlike the leaf economic spectrum, empirical patterns of fine-root trait variation and their relationship to plant strategies remain unclear. The complex pattern of trait covariation in fine roots likely arise due to the multi-dimensional nature of root trait expression, trait relationships with environmental conditions, and the influence of mycorrhizal associations. This study aims to understand the major influences on fine-root trait variation: taxonomy, mycorrhizal association, environmental conditions, and root-branching order. We conducted a hierarchical Bayesian analysis to assess how these factors influence morphological (root diameter, specific root length [SRL], and root tissue density [RTD]) and chemical (nitrogen, phosphorous, and calcium contents) root traits using the from the global Fine-Root Ecology Database (FRED v2.3).
After accounting for inherent variation in root traits among root orders within the root-branch hierarchy, we found that fine-root traits showed clear taxonomic and environmental signals, as well as tradeoffs among traits. Traits such as phosphorous content, RTD, and SRL varied less within species than across species. For example, the medians of standard deviation for standardized phosphorous content values (unitless) were 0.07 (intra-specific) and 0.11-0.48 (inter-specific, depending on mycorrhizal types). Intra-specific variation in many traits, especially morphological traits, was explained by significant association with environmental covariates (mean annual temperature and precipitation). However, the strength of environmental influence on intra-specific variation was small (e.g. taxonomy explained 88% of the variation in root phosphorous content, whereas environmental conditions only explained an additional 0.5%), although this could be related to insufficient within-species trait sampling across the representative range of environmental conditions. Moreover, different mycorrhizal associations modify the strength of the multivariate trait trade-offs across species, which may reflect different strategies for growth and competition belowground. These findings suggest that the major taxonomic-constrained trait groups and trade-off relationships provide a starting point for representing fine-root form and function in ecosystem models, and further investigation on how environmental conditions influence intra-specific variation is needed.

Title: Quantifying Terrestrial Drivers of Uncertainty in Earth System Model Predictions Using Machine Learning

Daniel M. Ricciuto,[1]* Dan Lu,[2] Anping Chen,[3] Jiafu Mao[1]

[1] Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2] Computational Sciences and Engineering Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[3] Department of Biology and Graduate Degree Program in Ecology, Colorado State University, Boulder, CO

Contact: (ricciutodm@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://tes-sfa.ornl.gov

Project Abstract: Climate scientists strive to improve predictive understanding of Earth system variability and change using models of ever-increasing mechanistic complexity and resolution. Continuing to improve such Earth system models (ESMs) will require increasing integration across several disciplines to determine key mechanisms and model parameters, where and when to place observations, the nature of impacts to human systems, and how to deal efficiently with large model output datasets. Uncertainty quantification (UQ) algorithms that use machine learning and artificial intelligence link observations and models together to produce credible simulations of Earth system behavior with uncertainty estimates. Deep neural networks (DNNs) combined with dimension-reduction techniques can be used to build fast-to-evaluate surrogate models of spatiotemporally varying model output fields using a smaller number of ESM ensemble members and higher accuracy than other methods. These surrogate models can then be used for uncertainty quantification techniques such as global sensitivity analysis, data assimilation or model calibration, leading to more rapid advances in model development, prediction of climate processes, and the design of new observation systems that are optimally suited to reducing model output uncertainties. Here we focus on uncertainty quantification of historical multi-site and global-scale predictions from the Energy Exascale Earth System land model (ELM) considering uncertainty in 12 key model parameters related to photosynthesis and water cycling. We constrain these model parameters using FLUXNET observations and present a new framework using surrogate models to calibrate using globally gridded remote sensing observations, including sun-induced fluorescence (SIF).

Title: Effects of Photosynthesis on the Timing of Autotrophic and Heterotrophic Respiration Fluxes

Melanie A. Mayes,[1*] Jeffrey D. Wood,[2] Junyi Liang,[1,3] Shikha Singh,[4] Sindhu Jagadamma,[4] Lianhong Gu,[1] Christopher W. Schadt[5]

[1]Environmental Sciences Division & Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]School of Natural Resources, University of Missouri, Columbia, Missouri;
[3]Department of Grassland Resources and Ecology, College of Grassland Science and Technology, China Agricultural University, Beijing, China;
[4]Department of Biosystems Engineering & Soil Science, University of Tennessee, Knoxville, TN;
[5]Biosciences Division & Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: (mayesma@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://tes-sfa.ornl.gov

Project Abstract: Resolving the contributions of heterotrophic and autotrophic respiration are key to improving ecosystem models and predicting future climates. The two kinds of respiration are intimately intertwined, due to the contributions of belowground root tissues and rhizosphere materials, aboveground litter contributions, and root exudates contributing simple organic compounds, all of which fuel microbial decomposition. Of the three components, only root exudates (photosynthate) change over diurnal cycles, but the impact on microbial respiration has not been determined. We will use long-term measurements of canopy sun-induced chlorophyll fluorescence observations as a proxy for canopy photosynthesis, and a 2-year trenching experiment equipped with continuous automated soil CO_2 efflux measurements to isolate heterotrophic from autotrophic respiration in soil at the Missouri Ozark AmeriFlux site in mid-Missouri. Recent studies have identified a 9-12-hour time lag between gross primary production and total soil respiration, but the components of soil respiration have not been deconvolved to understand the direct contribution of photosynthate to microbial respiration. This research will quantify the time lag between canopy photosynthesis and the components of soil respiration, and to determine how the dynamics of soil temperature and moisture, plant phenology, and physiological water stress modulate variations in the time lag, drawing on 2 years of field data. Lab-scale incubation experiments have focused on understanding the sensitivity of heterotrophic respiration to soil moisture. This work will contribute to understanding how above- and belowground processes are linked, and how they together respond to changes in phenology and weather.

Title: **Microbial Control Over Soil Carbon Saturation**

Matthew E. Craig,[1]* Melanie A. Mayes,[1] Benjamin N. Sulman,[1] Anthony P. Walker,[1]

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

Contact: (craigme@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://tes-sfa.ornl.gov

Project Abstract: Increasing soil carbon (C) storage is a key strategy to mitigate rising atmospheric CO_2, yet soil C pools often appear to approach a maximum value, or saturate, with increasing C inputs. The mechanisms underlying this phenomenon are poorly understood. Soil C saturation is commonly hypothesized to result from the finite amount of reactive mineral surface area available for forming mineral-associated C – the largest soil C pool in most systems. However, inputs to mineral-associated C are largely supplied by microbial activity, and the response of microbial biomass to C inputs might be limited by density-dependent factors – i.e. factors that alter growth or turnover as microbial density increases (e.g. competition or predation). Thus, we hypothesize that density-dependent constraints on soil microbial biomass represent an alternative or complementary mechanism by which soil C saturates. To evaluate this hypothesis, we first synthesized C addition studies to examine the premise that microbial biomass should exhibit a constrained, or sub-linear, response to increasing C inputs. We then explored the consequences of these microbial constraints by simulating microbial-explicit soil C models with alternative hypotheses about microbial growth and turnover in the multi-assumption architecture and testbed (MAAT). Our dataset – which contained more than 350 microbial biomass observations from *ca.* 100 C addition experiments – revealed a clear sub-linear relationship between organic input rates and soil microbial biomass. Based on ancillary measurements, we suggest that this constrained microbial biomass response was driven by less efficient growth or faster microbial turnover as C inputs and microbial biomass increased. Representing both of these effects in a three-pool soil C model led to saturation of the mineral-associated C pool but not the particulate C pool, a pattern often observed in saturation studies. Moreover, by manipulating the relative strength of growth versus turnover density-dependence, we were able to simulate three other previously observed saturation patterns: 1) insensitivity of particulate and mineral-associated C to inputs, 2) insensitivity of mineral-associated C with increasing particulate C, and 3) saturation of all soil C pools. Thus density-dependent controls on microbial growth versus turnover might differentially affect the response of soil C pools to increasing inputs. We conclude that soil C responses to altered C inputs – or indeed any environmental change – are likely influenced by the ecological factors that limit microbial populations. Considering these microbial constraints might better enable us to model soil C sequestration efforts.

Title: A Closed Model of Light Reactions of Photosynthesis for General Applications

Lianhong Gu,[1]* Joseph A Berry,[2] Albert Porcar-Castell,[3] Jimei Han,[4] Jeffrey D. Wood,[5] Christine Y-Y. Chang,[4] Ying Sun,[4] Yang C. Song,[6] Anthony P Walker,[1] David J Weston[7]

[1]Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN;
[2]Department of Global Ecology, Carnegie Institution of Washington, Stanford, CA;
[3]Department of Forest Sciences, University of Helsinki, Helsinki, Finland;
[4]School of Integrative Plant Science, Cornell University, Ithaca, NY;
[5]School of Natural Resources, University of Missouri, Columbia, MO;
[6]Hydrology and Atmospheric Sciences, University of Arizona, Tucson, AZ;
[7]Biosciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

Contact: (lianhong-gu@ornl.gov)
Project Lead Principal Investigator (PI): Paul J. Hanson
BER Program: TES
Project: TES SFA at Oak Ridge National Laboratory
Project Website: https://tes-sfa.ornl.gov

Project Abstract: Plants have evolved sophisticated mechanisms to balance the light and carbon reactions of photosynthesis as this match is vital to the normal functioning of the photosynthetic apparatus and long-term species survival. In theory, photosynthesis could be modeled from either the light or carbon reactions with a convergence expected. Historically, mechanistic modeling efforts have focused on the carbon reactions. This traditional focus is challenged in the era of growing interest in engineering crops for better photosynthetic efficiency and stress resilience and in using sun-induced chlorophyll fluorescence (SIF) to monitor photosynthesis at different scales; both efforts depend on our predictive capability on not just the carbon but also the light reactions. We have developed a closed system of light reactions that models photosynthesis, SIF and the balance between the light and carbon reactions with internal consistency. The closed system is formed by modeling the regulatory mechanisms of photosynthetic electron transport as a function of excess energy (the absorbed energy that cannot be dissipated photochemically) conditioned with the feedback effects of carbon reactions as influenced by temperature and CO_2 concentration. This solution embodies our understanding of the light reactions and is successfully tested against large datasets of fluorometry and gas exchange measured on a broadleaf deciduous and a needleleaf evergreen species across a wide range of environmental conditions. The closed system of light reactions eliminates circularity in photosynthesis estimation with SIF. It complements carbon reaction models to provide a framework for quantifying the light-carbon reaction balance to assist engineering crops with desired properties.

Title: **Accounting for carbon and energy edge effects in forest boundaries: A collaboration with ORNL, NIST, and Boston University**

Jeffrey Warren,[1,*] Melanie Mayes,[1] Peter Thornton,[1] Stan Wullschleger,[1]

[1]Oak Ridge National Laboratory, Oak Ridge, TN; [*]presenting author

Contact: (warrenjm@ornl.gov)

Project Lead Principle Investigator (PI): Melanie Mayes

BER Program: TES

Project: DOE Lab-led project (Oak Ridge National Laboratory)

Project Website: n/a

Project Abstract: The world's forests are highly fragmented, with 70% of forest area within a kilometer of an edge, and nearly 60% of North American forests within 100 m of an edge (Haddad et al. 2015). Forest edges as legacies of disturbance can have 50-100% greater productivity than the interior forest (Reinmann and Hutyra 2017). Yet, the increased productivity and changes in nutrient cycling, hydrology and soil carbon dynamics at forest edges are not well understood at the process level, and subsequently have not been adequately included in earth system modeling efforts. Beginning in 2016, researchers from Boston University and the National Institutes of Standards and Technology (NIST), began intensive, primarily aboveground ecophysiological observations of edge effects in a 67-ha forest remnant adjacent to meadow at the NIST campus in Gaithersburg, MD. In 2019, ORNL researchers added additional capacity with investigation of belowground hydrological, biogeochemical and biotic observations across meadow to interior forest transects, particularly soil C and nutrient concentrations, microbial and enzyme activities, autotrophic/heterotrophic respiration, root biomass and vertical profiles of soil water content and temperature. Results indicate increased rates of activity at the forest edge as compared with the interior forest and meadow locations. Soil pH declined and soil dissolved N and C increased from the forest interior into the meadow, and the large variation in NH4 and NO3 near the forest edge indicated some biological hotspots. While heterotrophic respiration dominated soil CO2 efflux across the transects, the forest edge and interior locations revealed a large autotrophic component that comprised 20% of total soil CO2 efflux. Throughout the soil profile, volumetric water content was driest at the forest edge and wettest 25 m away in the open meadow. In addition, there was strong evidence for hydraulic redistribution at the forest edge, based on a daily increase in water content in the absence of precipitation. Root trait distribution analysis is underway. Data will be used to test ELM and MEND model application to this unique interface, and to develop novel parameterization to improve representation of edges.

Haddad NM, et al. 2015. Sci Adv 1(2): e1500052

Reinmann, AB, Hutyra LR. 2017. Edge effects enhance forest carbon uptake. PNAS 114:107-112

Subsurface Biogeochemical Research

University Awards

Title: **Seasonal origins of tree water-use along a hillslope in the East River Watershed**

Max Berkelhammer[1*], Gerald Page[2], Christopher Still[2], Lauren Hildebrand[1], James Byron[1], Kelsey Foss[1].

[1]University of Illinois at Chicago, Chicago, IL;
[2] Oregon State University, Corvallis, OR;

Contact: berkelha@uic.edu

Project Lead Principal Investigator (PI): Max Berkelhammer

BER Program: SBR

Project: University Project: Space and time dynamics of transpiration in the East River watershed: biotic and abiotic controls (DE-SC0019210)

Project Abstract:

Transpiration is a key component of the hydrological budget of the East River Watershed (ERW). Unlike evaporation, which can be estimated with some confidence using energetic constraints, transpiration is more complicated to model due to complex dynamics associated with root distributions and the stomatal response to atmospheric forcing. To provide constraints for future modeling, we developed continuous transpiration fluxes for three key species in the ERW (*Picea engelmannii*, *Abies lasiocarpa* and *Populus tremuloides*) along a ~500 m hillslope transect during 2019-2020. The observations show that the conifers have the highest levels of transpiration in late May and early June followed by a long-term decline through the end of the growing season. This progressive decline is interrupted by a modest increase in early August associated with a series of summer rain events. The seasonal trend largely mirrors surface soil moisture. On the other hand, the aspens show two transpiration peaks of similar magnitude in early July and early August. The largest transpiration fluxes appear to be around 3200 m, which marks an intermediate elevation between water-limitation at lower elevations and temperature-limitation at upper elevations. While the temporal dynamics seem to largely be explainable by seasonal trends in soil moisture, a lag emerges in July between the time of day when transpiration reaches its peak and the period of highest atmospheric evaporative demand, which shows how the stomatal response to atmospheric conditions further modulate transpiration. In addition to the transpiration measurements, we also measured the water isotopic ratio of the xylem water to understand the water sources the trees relied on. As expected, the trees almost exclusively utilized snow melt early in the growing season. As the season progressed, some trees transitioned into use of precipitation while others continued to use snowmelt through the entire growing season. Interestingly, snowmelt reemerged as the predominant water source across the hillslope at the end of the season reflecting either use of deeper waters or that older waters had migrated into the root zone as evaporative demand increased. Ongoing work includes tree-level modeling of transpiration using the Soil-Plant-Atmosphere (SPA) model, continuing the sap flux and isotopic measurements through the 2020 growing season, adding canopy-scale thermal imaging of the canopy to better understand leaf level processes and making measurements of the metal content in the xylem water to separate the current season’s snow melt from groundwater.

Title: **The Hydro-bio-geochemistry of the Columbia River - Tributary Confluences**

Thomas Bianchi,[1*] David Butman,[2] Nicholas Ward,[2-3] Michael Shields,[4] Evan Arntzen,[5] James Stegen,[5] Julia Indivero,[3] Yulia Farris,[5] Albert Rivas-Ubach,[6] Nikola Tolic,[6] and Rosalie Chu[6]

[1]University of Florida, Gainesville, FL
[2]University of Washington, Seattle, WA
[3]Pacific Northwest National Laboratory, Sequim, WA
[4]Texas A&M University, College Station, TX
[5]Pacific Northwest National Laboratory, Richland, WA
[6]Environmental Molecular Sciences Laboratory, Richland, WA

Contact: (tbianchi@ufl.edu)

BER Program: SBR

Project: University Award: *The Influence of Microbial Priming Effects on the Hydro-bio-geochemistry in the Columbia River and its Tributary Confluences*

Project Website: Not applicable

Project Abstract:

River-tributary confluences, where diverse organic matter (OM) sources mix, are considered aquatic critical zones of biogeochemical cycling. The sources of OM to the Columbia River watershed are diverse, including dry land used for agricultural activity upstream from the McNary Dam and the Gifford Pinchot National Forest along the western reaches of the Cascades. Here we evaluate dissolved OM (DOM) composition and bioavailability in the mainstem of the Columbia River and four of its tributaries (Snake, Yakima, Walla Walla, and Wind rivers) in August 2018 and April 2019, respectively. We quantified concentrations of total dissolved organic carbon (DOC), total dissolved nitrogen (TDN), chromophoric dissolved organic matter (CDOM), dissolved lignin, dissolved hydrolysable amino acids, and examined the overall DOM molecular composition via Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR MS). DOC, TDN, and dissolved lignin concentrations were higher at most sampling locations in April when discharge was greater. Spatial and temporal variability in DOM composition was evident when examining the high-resolution mass spectrometry data along with the biomarker data via principal component analysis (PCA). For example, the Walla Walla River was relatively enriched in protein-like DOM in August but was enriched in dissolved lignin and phytochemical/oxyaromatic compounds in April. To assess bioavailability, field replicates and mixtures representing river-tributary confluences were incubated in the dark for 15 days. Total DOC significantly decreased only in a mixture representing the confluence of the Columbia and Walla Walla rivers sampled in August 2018. This was accompanied by a general decrease in dissolved lignin, but the decrease was not statistically significant. As mentioned above, the Walla Walla tributary was relatively enriched in protein-like DOM in August 2018. Therefore, it is possible this labile material primed the more stable Columbia River DOM. However, based on the insignificant decrease in dissolved lignin coupled with no significant changes in the compound class distribution measured via FT-ICR MS, the microbial community in the Walla Walla-Columbia mixture appeared to be indiscriminate of the molecular structure of the DOM.

Geophysical characterization of iron oxide precipitation in anoxic groundwater discharge zones

Chen Wang[1]*, Martin A. Briggs[2], Frederick D. Day-Lewis[2] and Lee D. Slater[1]

[1]Rutgers University, Newark, NJ;

[2]U.S. Geological Survey, Earth System Processes Division, Hydrogeophysics Branch, Storrs, CT;

Contact: (cw701@newark.rutgers.edu)

Project Lead Principle Investigator (PI): Martin A Briggs

BER Program: SBR

Project: University project

Project Website: (data releases)

http://doi.org/10.5066/P9Q1Z1TK; http://doi.org/10.5066/P9YWSJ2J; http://doi.org/10.5066/P931G95D

Project Abstract:

The precipitation of iron(III) oxides and/or hydroxides (Fe oxides) often occurs in streams and wetlands when low oxygen groundwater containing Fe(II) ions discharges into shallow oxygenated sediments and surface water. Efficient characterization of Fe oxide spatial distributions would permit identification of low oxygen groundwater discharge zones associated with contamination and enhanced biogeochemical reactions. Additionally, it would generate a better understanding of contaminant transport through river corridors as high surface area Fe oxides function as a sorption sink for dissolved contaminants (e.g., As, U). We aim to assess the spectral induced polarization (SIP) electrical geophysical technique for in situ and efficient characterization of Fe oxide precipitation in streambed sediments. We used laboratory experiments to show that the imaginary conductivity has a strong linear relationship (R^2=0.87) with sediment specific surface area, which in this case, is controlled by the concentration of fine-grained Fe oxides (up to 24.1 mg g^{-1}). We developed a specialized field measurement probe applied underwater to sense in situ the shallow streambed at up to 10 cm depth. We used a 1D analytical model to demonstrate the low sensitivity of the imaginary conductivity measurement to the electrically conductive stream water layer, a factor often complicating more typical electrical resistivity and electromagnetic measurements. We applied streambed SIP measurements along a coastal stream (Mashpee River, MA) and an alluvial river (East River, CO), where Fe oxide precipitates are formed by anoxic groundwater discharges resulting from a prior landfill leachate and beaver activities, respectively. We observed distinctly higher imaginary conductivity responses in the Fe oxide precipitation zones (up to 3 μS cm^{-1}) than the controlling background areas (generally less than 0.1 μS cm^{-1}). This study provides a new methodology for geolocating anoxic groundwater discharge zones and mapping spatial variations of sediment physicochemical properties.

The Effects of Stream Organic Matter on Respiration in Hyporheic Zones: Combined Insights from Flume and Computational Experiments

Anna Turetcaia[1], Bing Li[2], Xiaofeng Liu[2], Xingyuan Chen[3], Robert Danczak[3], Matthew Kaufman[3], Vanessa Garayburu-Caruso[3], Emily Graham[3], James Stegen[3], and M. Bayani Cardenas[1,*]

[1]The University of Texas at Austin, Austin, TX
[2]Pennsylvania State University, State College, PA
[3]Pacific Northwest National Laboratory, Richland, WA

(cardenas@jsg.utexas.edu)

BER Program: SBR
Project: University award

Hyporheic zones (HZs) are a critical part of river corridors because of high rates of biogeochemical reactions which take place in them. The most important of these reactions is aerobic respiration because it is thermodynamically favored and it helps set up the redox ladder. This project's goal is to improve the understanding of respiration in HZs. We ultimately seek predictive capabilities for the collection of HZ processes in system-scale models. The project is broadly divided into the intertwined tasks of advancing mechanistic models and the mapping and monitoring of reactions and the microbial communities responsible for these in real-scale laboratory flume experiments. Our most recent experiments are focused on determining how HZ respiration responds to perturbations in stream organic matter. In the flume, direct measurements of CO_2 production and O_2 consumption in both the overlying stream water and throughout the HZ sediment revealed that there is substantial respiration and that the rates vary with HZ depth. The experiments showed that the CO_2 in the stream, some of which is evaded to the atmosphere, is largely produced in the sediment and delivered to the channel by hyporheic exchange return flow. Computational flow and transport simulations, using the model we developed called *hyporheicFoam* which is based on the open-source model OpenFOAM, help explain the observed O_2 and CO_2 patterns. The simulations showed drastic gradients in the age of water flowing through the HZ. Most of the respiration happens in the shallowest HZ portion where the residence time is shortest and overlaps most with the respiration timescale and wherefrom the produced CO_2 is also easily expelled back to the stream. What therefore happened when stream organic matter increased was the respiration in the shallow HZ increased concurrently and linearly. As a consequence of the HZ-stream linkage, so too did the stream CO_2 concentration increase. Our study has shown that due to the strong coupling between the stream and the HZ, perturbations in stream dissolved organic matter are immediately felt within the HZ, which then quickly feedbacks to the stream. This new insight further highlights the importance of viewing the HZ and stream as a continuum, and that any predictive models will need to simultaneously and holistically consider these parts of the river corridor.

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

Jeffrey G. Catalano[1]*, Daniel E. Giammar[1], Jinshu Yan[1], Neha Sharma[1], Elaine D. Flynn[1], Grace E. Schwartz[2], Scott C. Brooks[2], Pamela B. Weisenhorn[3], Kenneth M. Kemner[3], Edward J. O'Loughlin[3], Daniel I. Kaplan[4]

[1]Washington University, Saint Louis, MO
[2]Oak Ridge National Laboratory, Oak Ridge, TN
[3]Argonne National Laboratory, Argonne, IL
[4]Savannah River National Laboratory, Aiken, SC

Contact: catalano@wustl.edu

Project Lead Principle Investigator (PI): Jeffrey G. Catalano

BER Program: SBR

Project: University Award

Project Abstract:

Biogeochemical cycling in subsurface aquatic systems is driven by anaerobic microbial processes. Many of the organisms involved mediate these processes using metalloenzymes that require trace metals as key reactive centers. Pure culture studies reveal that low availability of trace metals may inhibit methanogenesis, mercury methylation, and reduction of N_2O to N_2 during denitrification. However, whether such limitations occur in natural subsurface aquatic systems is currently unclear. If present, such limitations are likely controlled by trace metal speciation as this directly impacts bioavailability. This project seeks to establish mechanistic links between trace metal availability and biogeochemical carbon, nitrogen, and mercury transformations in subsurface systems. Integrated field and laboratory studies of trace metal availability and biogeochemical processes are underway at riparian wetlands in the Tims Branch watershed at the Savannah River Site and marsh wetlands at Argonne National Laboratory, both in collaboration with the Argonne Wetland Hydrobiogeochemistry SFA, as well as the streambed of East Fork Poplar Creek (EFPC) at Oak Ridge National Laboratory in collaboration with the ORNL Mercury SFA. Solid-phase trace metal (Co, Ni, Cu, Zn) concentrations in the soils and sediments at these sites are one-half to one-tenth of crustal averages. The overlying surface waters have dissolved trace metal concentrations roughly an order of magnitude below optimal levels for microbial processes. These observations suggest that our field sites will display metal-limited biogeochemistry. Despite the distinct physical settings under investigation, the speciation of trace metals in the wetland soils and stream sediments varied little, suggesting broadly universal controls on metal availability in subsurface aquatic systems. While the wetland soils and stream sediments displayed similar trace metal uptake behavior, added metals surprisingly formed different species at each site. Cobalt addition to stream sediments did not produce a clear impact on mercury methylation, but further studies are needed to examine longer incubation times. Ongoing incubations of wetland soils and stream sediments are investigating whether the addition of nickel and copper stimulate methanogenesis and N_2O reduction, respectively.

Title: **Subalpine forest regeneration decreases DOM exports, but increases DOM reactivity to headwater streams**

Tim Fegel[1]*, Claudia Boot[2], Tim Covino[2], Kelly Elder[1], Ed Hall[2], Banning Starr[1], James Stegen[3], Charles Rhoades[1]

[1]U.S. Forest Service, Rocky Mountain Research Station, Fort Collins, CO
[2]Colorado State University, Fort Collins, CO
[3]Pacific Northwest National Laboratory, Richland, WA

***Corresponding Author Contact Information:**
U.S. Forest Service, Rocky Mountain Research Station 240 W. Prospect, Fort Collins, CO, 80526
Tel: 970-498-1017 email: timothy.fegel@usda.gov

Project Lead Principal Investigator (PI): Tim Covino

BER Program: SBR

Project: University project, Quantifying hydro-biogeochemical controls on watershed dissolved organic matter flux and processing

Project Abstract: The headwater forest ecosystems of the western U.S. generate a large portion of the dissolved organic matter (DOM) transported across North America. Land cover type, specifically tree species composition and structure in these headwater forests affect the quantity and characteristics of DOM transferred from terrestrial to aquatic ecosystems. Disturbance and management reset headwater forest species composition, with lasting effects on watershed carbon cycling. We investigated the role of forest land cover change between old growth and regenerating second-growth subalpine forest hillslopes in regulating the character and reactivity of DOM. Inputs of DOM derived from litter leachates and exports of DOM from lateral subsurface flow at the base of trenched hillslopes were evaluated during a three-year period (2016-2018) at the Fraser Experimental Forest in northcentral Colorado, USA. Differences in land cover type between old-growth and regenerating forest correlated with changes in DOM composition and reactivity. Subsurface flow draining the old-growth forest was higher in dissolved organic carbon (DOC) and total dissolved nitrogen (TDN). DOM composition from the old-growth forest had higher C:N ratio and was molecularly more complex and more aromatic than DOM from regenerating forest. DOM derived from the second-growth forest was more consistent with signatures of microbial processing. DOM from the second growth forest also had significantly higher biological oxygen demand (BOD) compared to the old-growth forest. Our findings demonstrate that changes in forest species composition and associated litter alter the composition and reactivity of DOM from liter and exports to adjacent aquatic ecosystems. Mixtures of old-growth and second-growth forests are common across headwater landscapes, and this study elucidates how these forest types drive a coupling between the composition and reactivity of DOM transferred from terrestrial to aquatic ecosystems.

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

Jeffrey S. Deems,[1,2] Mark Raleigh,[1] Gabriela Collao-Barrios,[1]

[1] CIRES National Snow and Ice Data Center, University of Colorado, Boulder, CO;
[2] CIRES NOAA Western Water Assessment, University of Colorado, Boulder, CO;

Contact: (deems@nsidc.org)

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

BER Program: SBR

Project: University project

Project Abstract:

Spatial and temporal patterns of snow accumulation and melt exert a dominant control on hydrologic and biogeochemical flows in temperate mountain catchments. Mountain snowpack states, fluxes, and properties exhibit extreme and scale-dependent variability, complicating efficient sampling and modeling. Capabilities for evaluating the impacts of system perturbations (e.g. climate shifts, radiative forcing by impurities, forest cover change) on system water availability and nutrient cycling are contingent on robust observations and simulations of seasonal snow dynamics at appropriate scales of action.

To explore snow accumulation and melt process dynamics over the meter to watershed scales, we have implemented a physically-based snow cover evolution model (SnowModel; Liston et al., 2006) at multiple grid resolutions, using different combinations of accumulation process sub-models. We first tested the model in Senator Beck Basin, a well-instrumented study site in southwest Colorado. Model parameterizations for that site were then transferred to the East River SFA where instrumentation is less-reliable.

The simulations over a recent set of years spanning high and low peak accumulation values, were forced with high-resolution mesoscale model (WRF) and data assimilation model (HRRR) output, and are compared with ground measurements as well as snow depth and snow water equivalent (SWE) maps from Airborne Snow Observatory flights. These results help characterize the snow hydrologic system in the East River, and set the stage for future snow data assimilation work and for integration with simulations of connected systems within the SFA.

References:

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

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

Jason Demers[1*], Joel Blum[1], Scott Brooks[2], Elizabeth Crowther[1] [1]University of Michigan, Ann Arbor, MI [2]Oak Ridge National Laboratory, Oak Ridge, TN

(jdemers@umich.edu)

Project Lead Principal Investigator (PI): Jason D. Demers BER Program: SBR
Project: University-Led Research Project Website: n/a

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 suggest that additional dissolved Hg from the hyporheic pore water or groundwater discharge may variably contribute as much as a third of downstream dissolved Hg loads during baseflow conditions. Thus, the over-arching goal of this project is to use natural Hg stable isotope signatures, imparted by molecular-scale reactions, to gain a more comprehensive quantitative and mechanistic understanding of the processes that supply dissolved Hg to surface water, drive observations of watershed-scale Hg fluxes, and result in bioaccumulation of methylmercury (MeHg).

To achieve this goal, we are combining a multi-seasonal field study with mechanistic laboratory experiments. First, we are coupling the Hg isotopic composition of dissolved Hg in stream water and in critical subsurface ecosystem compartments (i.e., hyporheic zone, riparian floodplains, and groundwater) with hydrologic fluxes in four reaches of EFPC to establish an isotope mass balance that assesses the relative importance of dissolved Hg contributed to the stream across these critical interfaces. Second, we are utilizing sequential extraction methods to characterize the isotopic composition of legacy Hg potentially re-mobilized from streambed sediment. This will provide insight into the sources and mechanisms that replenish the supply of dissolved Hg within critical subsurface zones. Third, we are assessing the isotopic composition of MeHg in biota of EFPC, as a step toward identifying the source(s) of bioaccumulative MeHg in the EFPC ecosystem.

Here, we present: (1) Hg concentration and isotopic composition of surface water, hyporheic pore water, and riparian groundwater; (2) isotopic mass balance assessments regarding legacy inputs of dissolved Hg to stream water of EFPC; and (3) Hg isotopic composition of sequentially extracted Hg from streambed sediment. We provide an overarching synthesis that shows: (*i*) recalcitrant fractions of legacy Hg in sediment is likely contributed to dissolved pore water and stream water; (ii) soluble sediment Hg fractions are likely derived from periphyton; and (iii) recalcitrant Hg released from legacy sediment may be incorporated into more soluble periphyton materials downstream along the flow path.

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

Jennifer L. Druhan[1*], Alison Tune,[2] Jia Wang[1], Corey R. Lawrence[3], Jiamin Wan[4], Daniella Rempe[2]

[1]Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA;
[2]Jackson School of Geosciences, University of Texas at Austin, Austin, Texas, 78705, USA;
[3]U.S. Geological Survey, Denver, Colorado 80225, USA;
[4]Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA

Contact: jdruhan@illinois.edu

Project Lead Principal Investigator (PI): Jennifer L. Druhan

BER Program: SBR

Project: University project

Project Abstract: In upland forested hillslopes such as the East River watershed, roots extend well beneath the classically defined soil layer into partially weathered, unsaturated rock to access both water and nutrients. Yet current carbon cycle models rarely extend below shallow soils, and the contribution of this deeper subsurface nutrient cycling to carbon stocks and fluxes is virtually unknown. In the Eel River watershed of Northern California, a team of SFA collaborators have successfully installed a novel Vadose zone Monitoring System (VMS) consisting of a pair of sub-horizontal bore holes instrumented with flexible plastic sleeves which allow sampling of fluids draining through the partially saturated shale weathering profile, as well as gas sampling ports, moisture and temperature sensors. Using this unique instrumentation, a DOE-SBR exploratory project (PI Druhan, DE-SC0019198) is now constraining carbon stocks and fluxes as an analog to the hillslopes of the East River, which is similarly underlain by a shale lithology and hosts mature forest ecosystems. These data provide new evidence that approximately 30% of net CO_2 flux from the terrestrial environment to the atmosphere is sourced many meters below the soil layer (see A. Tune student poster for further details). Critically, the exploratory DOE-SBR grant has now shown that this CO_2, though produced many meters below the soil, is radiocarbon modern. Thus, in total, this work indicates that modern carbon is being delivered rapidly to the deep subsurface, likely as a result of deep rooting zones, and this previously undocumented carbon cycle is a substantial component of the CO_2 generated in the terrestrial environment. To extend these results, we have constructed a radioisotope-enabled version of the CrunchTope software which is now benchmarked as part of the exploratory proposal awarded to Dr. Druhan (Druhan et al., 2020). The new model is capable of simultaneous and explicit simulation of the three isotopes of carbon including both stable isotope fractionation and radioactive decay. Through this advanced modeling capability, the rates of carbon oxidation, contribution to weathering and thus the development of soils and sustainability of forest ecosystems will be embedded within an adaptive and predictive model framework.

Druhan, J.L.; Guillon, S., Lincker, M.; Arora, B. (2020) Stable and radioactive carbon isotope partitioning in soils and saturated systems: A reactive transport modeling benchmark study. *Computational Geosciences,* in press.

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

Christian Dewey,[1*] Rene Boiteau,[2] Marco Keiluweit,[3] Scott Fendorf[1]

[1]Stanfored University, Stanford, CA; [2]Oregon State University, Corvalis, OR; [3]University of Massachusetts; Amherst, MA

Contact: Fendorf@stanford.edu

Project Lead Principal Investigator (PI): Scott Fendorf BER Program: SBR

Project: University Project

Project Abstract: Dissolved organic matter (DOM) has a major but poorly understood control over the mobility of metals in surface and subsurface systems. Variations in the chemical composition of DOM across watersheds, owing to divergent organic matter transformation pathways, have potentially important influences on metal mobility. An outcome that has largely remained unexplored, but which may have critical impacts on dissolved metal concentrations and associated migration, is variation in the functional composition of DOM.

The ***overarching goal*** of our project is to determine the effect of redox conditions resulting from differing hydrologic environments on formation and transport of soluble metal-organic complexes. To meet our research goal, we developed a method to separate and quantify organic- metal complexes in natural DOM. We evaluated the role of column chemistry and solvent composition on elution and recovery of complexes of metals ranging in binding preferences (Al, Fe, Co, Ni, Cu, Zn, Cd, Pb) with (i) Suwannee River NOM and (ii) Suwannee River Fulvic Acid. Further, we examined variations in organic ligand binding of Cd from the DOE-sponsored East River Watershed using LC-ICPMS. Floodplain sediment pore-water samples were collected from oxic and anoxic environments and reacted with Cd. We observed significant differences in the composition of Cd binding ligands. In the oxic samples, three distinct Cd peaks are observed at early retention times, indicating different polar species. In the anoxic sample, the polar species are far less abundant and nonpolar ligands are observed. These results lead us to posit that redox environment, controlled by hydrologic state, is a major control over the composition of organic ligands across different regions of the watershed, and is consistent with the recent findings on the broader composition of organic matter across redox zones.

Our work is advancing a process-based understanding of metal fate and transport within watersheds, focusing principally on the dynamic hydrologic states of floodplains, leveraging the Columbia River, East River and Savannah River watersheds as experimental testbeds. Ultimately, our work is helping to advance the SBR programs goal of developing a robust predictive understanding of how hydrologic changes in watersheds affect water quality and inorganic element/contaminant loading.

Title: Metagenomic Insights into Key Nitrogen-Cycling Microbial Taxa within the Terrestrial Subsurface at Riverton, WY

Christopher A. Francis[1]*, Linta Reji[1], Emily L. Cardarelli[1], Bradley B. Tolar, John R. Bargar[2], and Nicholas Bouskill[3]

[1] Department of Earth System Science, Stanford University, Stanford, CA
[2] SLAC National Accelerator Laboratory, Menlo Park, CA
[3]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: caf@stanford.edu

Project Lead Principal Investigator (PI): Christopher Francis

BER Program: SBR

Project: University project DE-SC0019119

Project Abstract: Naturally-reduced zones (NRZs), formed within contaminated DOE legacy site floodplains in the upper Colorado River Basin, contain large inventories of nitrogen (N) and uranium (U). Microbial N-cycling processes, like nitrification and denitrification, have the capability to "unlock" the biogeochemical nutrient supply stored within NRZs, drive carbon cycling, and liberate U to the aquifers. However, despite their biogeochemical importance, remarkably little is known regarding N-cycling microbial communities within terrestrial subsurface sediments, let alone NRZs. To address this knowledge gap, we have performed detailed metagenomic analysis of microbial communities within sediment samples collected from the Riverton, WY subsurface. In particular, we have employed cutting-edge 'binning' approaches to generate metagenome-assembled genomes (MAGs) from 12 subsurface depths within a ~2.4 m sediment depth profile. This resulted in the generation of 100s of draft- to high-quality MAGs, many of which correspond to N-cycling taxa. Since our recent work highlighted the importance of ammonia-oxidizing archaea (AOA) in the Riverton subsurface (based on N-cycling functional genes and 16S rRNA amplicon sequencing), a major goal of this project was to definitively link key AOA functional genes (e.g., *amoA*, *nirK*, etc.) to their corresponding 16S rRNA sequences through the analysis of thaumarchaeal MAGs. Our binning efforts resulted in over 20 distinct thaumarchaeal MAGs spanning 11 different depths. Phylogenetic analysis of these genomes, based on ribosomal proteins and multiple functional genes, revealed truly remarkable AOA diversity. Interestingly, comparison of these MAGs to reference genome sequences revealed that, while some genomes were most closely related to known terrestrial AOA (e.g., *Nitrososphaera*, *Nitrosocosmicus*), others either represent completely novel lineages or are most closely to AOA from aquatic and even marine environments. We also observed islands of AOA gene clusters unique to Riverton MAGs. Interestingly, pangenome analysis revealed a clear distinction between AOA genomes derived from 'above' versus 'below' the water table, highlighting the underappreciated importance of hydrology in controlling AOA distribution and diversity in this environment. Finally, several nitrite-oxidizing bacterial genomes (e.g., *Nitrospirota*) were also obtained (containing *nxr* genes), which likely oxidize the nitrite produced by AOA to nitrate in these sediments. Overall, this project is yielding unprecedented genomic and ecophysiological insights into the microbial communities responsible for N-cycling, and especially nitrification, in a terrestrial subsurface environment that is directly influenced by hydrological fluctuations.

Physical, Biological and Resource Supply as Key Factors Driving Nutrient Uptake Along a Fluvial Network

Jancoba Dorley[1*], Ricardo González-Pinzón[1], Dave Van Horn[2]

[1]Department of Civil, Construction and Environmental Engineering, University of New Mexico, Albuquerque, New Mexico
[2]Department of Biology, University of New Mexico, Albuquerque, New Mexico

Contact: (gonzaric@unm.edu)

Project Lead Principal Investigator (PI): Ricardo González-Pinzón

BER Program: SBR

Project: University Project

Project Abstract: Nutrient impairment has led to damages to US surface and groundwater systems in excess of 100 billion dollars per year. Therefore, there is a strong need to develop methods to predict the transport, uptake, and export of nutrients along fluvial networks. We present results that are based on a data-driven mechanistic understanding of three factors that largely control nutrient uptake and export: 1) interactions between transport-related processes (mass transfer to metabolically active zones), 2) resource supply dynamics (nutrient concentration, Stoichiometric constraints, etc.), and 3) biological controls (microbial community structure and function). Our results were generated from column experiments conducted along the Jemez River-Rio Grande continuum which spans four orders of magnitude in mean annual discharge, more than 2000 m in altitude, and more than 500 km of stream longitude. Two resource supply injections were performed on each of the columns, i.e., a nitrate only addition, followed by a stoichiometrically 'balanced' 106Carbon:16Nitrogen:1Phosphorus addition. We quantified NO3-N uptake kinetics while constraining three variables: stream order, sediment type and type of injection(N vs stoichiometrically 'balanced' C:N:P) throughout the river continuum. We observed increases in NO3-Nuptake velocity for the Stoichiometrically 'balanced' injection relative to concentrations during the Nitrate only injection, except for the 1stand one of the 7thOrder sites (downstream of a Wastewater Treatment Plant). Higher NO3-N uptake velocities were also observed in the Native sediment compared to the sterile sediments. We also observed that limitation and co-limitation in biological NO3-N across the two-injection experiments varied with stream order. Lastly, the Michaelis-Menten asymptotic decay pattern was observed for NO3-N uptake kinetics. While our results shows that stoichiometric imbalances limits nutrient uptake in lotic systems, ongoing work with our partners at the Pacific Northwest National Laboratory (PNNL) is seeking to identify how the type of microbial communities sampled from each of the columns control the observed uptake results.

Resolving Aquifer Controls on Larger River-Groundwater Exchanges of Mass and Energy

Michael Gooseff[1]*, Xingyuan Chen[2], Martin Briggs[3], Neil Terry[3], Evan Arntezn[2]

[1]University of Colorado, Boulder, CO;
[2]Pacific Northwest National Laboratory, Richland, WA;
[3]Hydrogeophysics Branch, US Geological Survey, Storrs, CT;

Contact: michael.gooseff@colorado.edu

Project Lead Principle Investigator (PI): Gooseff
BER Program: SBR
Project: University Project

Streams and rivers exchange water with surrounding aquifers preferentially through permeable geologic units. These exchanges of water between the surface and subsurface are important vectors of energy, biota, and solutes. They support fisheries and the removal of some pollutants from rivers. When submerged they are invisible to the naked eye, and to date, we have a poor understanding of the geologic controls on these exchanges in large river settings, hampering the development of predictive models. The overarching goal of this research project is to determine whether the dominant controls on groundwater inflows to rivers lie at the bed of the river or underneath the riverbed. Riverbeds are rarely smooth, regardless of their make-up (fine sediment versus gravel). Bedforms are generated in patterns that reflect the energy of the moving water in the channel. Across these bedforms, moving river water experiences shear stress, which can "pump" water into and out of the riverbed. Beyond the riverbed and its shorelines, the geologic setting of a river strongly dictates the river form (sinuosity and slope for example), as well as the potential patterns of water movement between the surface and subsurface. Current work along the Columbia River corridor being completed by scientists at the Pacific Northwest National Laboratory includes modeling convective exchange of river water through the bed and banks, broader groundwater flow modeling, and the collection of shallow geophysics data to characterize the distribution of near-surface geologic deposits that might influence river-groundwater exchange. In this research, we seek to identify groundwater inflows to the Columbia River using established and emerging field techniques adopted for large channels, and determine whether they are associated with the geologic structure around the river or the convective exchange along the riverbed. We will collect deep geophysical data using a FloaTEM system, which is a new cutting-edge tool for towed investigations.

This research will significantly complement the PNNL Scientific Focus Area research project on river corridors. Our findings will help put into context the processes occurring immediately adjacent to river channels, and help discriminate between proximal and distal controls. Our findings will also be useful for informing and calibrating reactive transport models being developed by other science groups working along the Hanford Reach of the Columbia River. The findings will also advance our fundamental understanding of the connections of landscapes to large river systems, which has potentially significant implications for water and fisheries management practices.

Title: **Methylation Potential of Mercury for Different Groups of the Methylating Microbial Community**

Heileen Hsu-Kim[1], Natalia Neal-Walthall[1], Austin Wadle[1], Caitlin M. Gionfriddo[2], Dwayne Elias[2], Cynthia C. Gilmour[3]
[1] Duke University, Department of Civil & Environmental Engineering, Durham, NC
[2] Oak Ridge National Laboratory, Oak Ridge, TN
[3] Smithsonian Environmental Research Center, Edgewater, MD

Contact: (hsukim@duke.edu)

Project Lead Principal Investigator (PI): Heileen Hsu-Kim

BER Program: SBR

Project: University project

Project Website: N/A

Project Abstract:

Methylmercury (MeHg) is a highly bioaccumulative form of mercury (Hg), and the mitigation of risk at contaminated sites requires tools to quantitatively predict MeHg production. This study examined the factors influencing microbial methylation of mercury (Hg) in freshwater wetland ecosystems with the goal of developing geochemical and biomolecular markers for net MeHg production potential. We are testing the hypothesis that mercury methylation potential in sediments can be predicted through a combination of diffusive gradient in thin-film (DGT) passive samplers (for bioavailable Hg flux) with genomic analysis of Hg-methylating microbial communities. We constructed three simulated freshwater wetlands in an outdoor field research station at Duke University. Each mesocosm comprised a $3.7\times1.2\times0.8\ m^3$ (length×width×height) slant-bottom box, filled with soil and water to create a gradient of water saturation conditions and was populated with freshwater macrophytes, mosquitofish, and associated macrofauna. After establishment of the simulated wetlands, each mesocosm box was amended with four different geochemically relevant and isotopically labelled inorganic Hg species to represent a gradient of different Hg methylation potentials across the four isotopes. Over several months, after the initial spike of mercury forms in the wetland mesocosms, we monitored each isotopically labelled Hg endmember for: (1) Accumulation into water, sediment and biological components in the mesocosm; (2) Conversion to MeHg in water and sediments; and (3) Accumulation of total Hg and MeHg on DGTs deployed for one week periods in the mesocosms. The results showed that most of the added Hg from each isotope accumulated in the top few centimeters of surface sediment in the first month after dosing. Greater conversion to MeHg was generally observed for the isotopes originating from dissolved forms ($^{202}Hg^{2+}$, ^{201}Hg-humic acid complex) than for isotopes originating from particulate forms (nanoparticulate ^{200}HgS and ^{199}Hg adsorbed to FeS). Also, the uptake of inorganic Hg in DGTs were generally consistent with trends for methylated Hg, indicating that DGT passive samplers might be useful as an empirical tool to evaluate Hg bioavailability for methylating organisms. Ongoing work will attempt to establish changes in the sediment microbial community during the 12-month period after Hg dosing, and compare to the observed changes in the extent of Hg methylation during this time frame.

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

Marco Keiluweit[1]*, Zoe G. Cardon[2], Malak Tfaily[3], Hui Li[1], Mariela Garcia-Arredondo[1], Rosalie Chu[4], Rene Boiteau[5], Yilin Fang[6], Steve Yabusaki[6]

[1]University of Massachusetts, Amherst, MA [2]Marine Biology Laboratory, Woods Hole, MA [3]University of Arizona, Tucson, AZ
[4]Environmental Molecular Science Laboratory, Richland, WA
[5]Oregon State University, Corvallis, OR
[6]Pacific Northwest National Laboratory, Richland, WA

Contact: (keiluweit@umass.edu)

Project Lead Principal Investigator (PI): Marco Keiluweit

BER Program: SBR

Project: University project (exploratory)

Project Website: NA

Project Abstract: Biogeochemical cycles within mountainous watersheds are key regulators of ecosystem carbon storage and downstream nutrient loadings, and they have shown to be particularly vulnerable to climate change impacts. Increasing temperature and persistent droughts have already dramatically changed vegetation cover across the mountainous western US, with unknown consequences for carbon and nutrient cycles in soils belowground. What remains elusive is to what extent associated changes in root-soil interactions may mobilize the vast pool of organic matter (OM) that has been stabilized by associations with minerals for centuries or millennia. Although plant root-driven OM mobilization from minerals may be a central control on carbon loss and nutrient export, such mechanisms are currently missing from conceptual and numerical models. The *overall objective* of this project is to identify the biogeochemical mechanisms by which roots destabilize mineral-OM associations and the cumulative impact on carbon and nutrient fate. To accomplish this goal, we integrated model system and greenhouse experiments with a scalable modeling approach. We conducted ***model system experiments*** to assess the vulnerability mineral-associated organic matter (MAOM) to exudate-mediated mechanisms. Our results show that common root exudates effectively destabilize MAOM not only through direct, ligand-driven mobilization mechanisms, but also indirect, microbially-mediated mechanisms relying on secondary metabolites and enzymes. We further found that OM bound to poorly crystalline Fe and Al (hydr)oxides is more vulnerable to exudate-induced destabilization than OM bound to more crystalline phases, particularly in response to direct, ligand-promoted mechanisms. These findings demonstrate that the stability of MAOM is not just a function of their inherent properties, but also will depend in large parts on the ability of plant roots and microbes to produce exudates capable of triggering suitable mobilization mechanisms. We further employed a well-controlled ***rhizobox approach***, combined with advanced microsensor and mass spectrometry techniques, to resolve spatiotemporal variations in the composition and availability of exudates along single growing roots of grasses. We show that the composition of functionally relevant exudate compounds varies at extremely short time scale, seemingly shifting from ligands such as aromatic acids around root tips to less reactive metabolites such as amino acids around mature root segments. These results suggest a prevalence of direct MAOM mobilization mechanisms around the root tip, while indirect MAOM mobilization strategies may dominate around more mature root segments. Finally, employing parallel microsensor measurements of moisture, redox, oxygen, and pH dynamics in the rhizosphere, we ***parameterized a rhizosphere (hydro)biogeochemistry reactive transport model***. The resulting model was used to assess how transient changes in (hydro)biogeochemical properties of the rhizosphere affect that stability of MAOM. Simulations suggest that diel pulses in root exudation are strong enough to significantly destabilize MAOM. We will further

highlight ongoing field-based experiments aiming to quantify the impact of MAOM mobilization across the subalpine East River watershed. In sum, results from our integrated experiment-modeling project highlights the strong control plant roots exert on the stability of MAOM and, thus, on the potential for carbon and nutrient export from watersheds.

Title: **Watershed scale seismic imaging and porosity estimation with the seismic land streamer in the Upper East River, Colorado**

James St. Clair[1], Lee M. Liberty[1]

[1]Boise State University, Boise, ID

Contact: (lliberty@boisestate.edu)

Project Lead Principal Investigator (PI): Lee Liberty

BER Program: **SBR**

Project: Boise State award DE-SC0019224

Project Abstract:

The East River Watershed Science Focus Area is a DOE funded experimental watershed dedicated towards developing a predictive understanding of hydrologic and biogeochemical processes within mountain watersheds. Bedrock in the watershed is composed of Mancos Shale and younger crystalline intrusions. Hillslopes are mantled with weathered bedrock, moraines, landslides and colluvium. During October of 2018 we conducted a watershed scale seismic survey of the drainage. The dataset includes ~12 km of data collected along roads with a 72-channel, 1.25m spaced streamer and ~3km of planted geophone data. P-wave (Vp) and shear wave (Vs) results reveal a sharp transition between regolith/sediment deposits and bedrock throughout the watershed. This sharp velocity contrast produces a high amplitude secondary arrival, which travels at the expected bedrock Vs. We interpret this arrival as a vertically polarized shear wave and use it to constrain bedrock Vs. Mancos Shale Vp anisotropy is measureable in some parts of the watershed and notably absent in the vicinity of crystalline intrusions. This suggests contact metamorphism influences bedrock hydrology. Hertz-Mindlin derived porosity estimates measurements show relatively high porosities within alluvial and colluvial (up to 0.5) deposits compared to bedrock (less than 0.05), in agreement with borehole observations. Localized, low Vp anomalies in the bedrock correlate with regional fracture sets visible in Lidar data, however their limited vertical extent suggests that permeability along these fractures decreases rapidly with depth. We also observe bedrock Vp trends that correlate strongly with local shale dip, bedrock Vp is slowest where the Mancos Shale dips into hillslopes and fastest where the shale dip is parallel to the hillslope. These results suggest shale structure strongly influences bedrock hydrology.

Distinct Source Water Chemistry Shapes Contrasting Concentration-Discharge Patterns[a]

Wei Zhi[1], Li Li[2], Wenming Dong[3] , Wendy Brown[4] , Jason Kaye[5], Carl Steefel[3], Kenneth H. Williams[3,4]

[1]Department of Energy and Mineral Engineering, The Pennsylvania State University, University Park, PA
[2]Department of Civil and Environmental Engineering, The Pennsylvania State University, University Park, PA
[3]Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, CA
[4]The Rocky Mountain Biological Laboratory, Crested Butte, CO
[5]Department of Ecosystem Science and Management, The Pennsylvania State University, University Park, PA

Project Lead Principal Investigator (PI): Li Li, SBR University project DE-SC0016221, collaboration with the Watershed Function Science Focus Area at Lawrence Berkeley National Laboratory funded by the DOE SBR under the contract DE-AC02-05CH11231

Project Website: Li Reactive Water Group

Contact: (lili@engr.psu.edu)

Abstract Understanding concentration-discharge (C-Q) relationships are essential for predicting chemical weathering and biogeochemical cycling under changing climate and anthropogenic conditions. Contrasting C-Q relationships have been observed widely, yet a mechanistic framework that can interpret diverse patterns remains elusive. This work hypothesizes that seemingly disparate C-Q patterns are driven by switching dominance of end-member source waters and their chemical contrasts arising from subsurface biogeochemical heterogeneity. We use data from Coal Creek, a high-elevation mountainous catchment in Colorado, and a recently developed watershed reactive transport model (BioRT-Flux-PIHM). Sensitivity analysis and Monte-Carlo simulations (500 cases) show that reaction kinetics and thermodynamics and distribution of source materials across depths govern the chemistry gradients of shallow soil water and deeper groundwater entering the stream. The alternating dominance of organic-poor yet geo-solute-rich groundwater under dry conditions and organic-rich yet geo-solute- poor soil water during spring melt leads to the flushing pattern of dissolved organic carbon and the dilution pattern of geogenic solutes (e.g., Na, Ca, and Mg). In addition, the extent of concentration contrasts regulates the power law slopes (b) of C-Q patterns via a general equation $b = \frac{\delta_b C_{ratio}}{C_{ratio,1/2} + C_{ratio}} + b_{min}$. At low ratios of soil water versus groundwater concentrations ($C_{ratio} = C_{sw} / C_{gw}$) < 0.6), dilution occurs; at high ratios ($C_{ratio} > 1.8$), flushing arises; chemostasis occurs in between. This equation quantitatively interprets b values of 11 solutes (dissolved organic carbon, dissolved P, NO_3, K, Si, Ca, Mg, Na, Al, Mn, and Fe) from three catchments (Coal Creek, Shale Hills, and Plynlimon) of differing climate, geologic, and land cover conditions. This indicates potentially broad regulation of subsurface biogeochemical heterogeneity in determining C-Q patterns and wide applications of this equation in quantifying b values, which can have broad implications for predicting chemical weathering and biogeochemical transformation at the watershed scale.

Reference:

[a] Zhi, W.; Li, L.; Dong, W.; Brown, W.; Kaye, J.; Steefel, C.; Williams, K. H., Distinct Source Water Chemistry Shapes Contrasting Concentration-Discharge Patterns. *Water Resour. Res.* **2019,** *55*, (5), 4233-4251.

Development of a molecularly informed biogeochemical framework for reactive transport modeling of subsurface carbon inventories, transformations and fluxes

Kate Maher[1*], Matthew J. Winnick[1,2], Dana K. Chadwick[1], Hsiao-Tieh Hsu[1],Yuchen Liu[3], Jennifer L. Druhan[3], Corey R. Lawrence[4]

[1] Department of Earth System Science, Stanford University, Stanford, California 94305, USA
[2] Department of Geosciences, University of Massachusetts Amherst, Amherst, MA 01003
[3] Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA
[4] U.S. Geological Survey, Denver, Colorado 80225, USA

Contact: kmaher@stanford.edu

Project Lead Principal Investigator (PI): Kate Maher

BER Program: SBR

Project: University Project

Project Abstract: Soils moderate the two largest fluxes in the carbon cycle: plant uptake of atmospheric CO_2 through photosynthesis and the resulting heterotrophic and autotrophic respiration that returns CO_2 to the atmosphere. Imbalances in these fluxes can thus substantially alter global carbon budgets and promote positive feedbacks in the climate system that are not well resolved in large scale climate models. The flux of carbon between the vegetation and the atmosphere is moderated by the soil organic carbon (SOC) reservoir, which is highly sensitive to shifts in (1) water availability and (2) vegetation dynamics. To address the potential for moisture-driven feedbacks, the overarching goal of our project is to develop new techniques to quantify soil organic carbon transformations that support development of new models of carbon (and nutrient) transfers to and from the soil reservoir.

To quantify the controls on depth-resolved net CO_2 production rates and the spatial variability in SOC inventories and guide model development, we are using field measurements of soil respiration, soil $p$$CO_2$ and SOC content in tandem with remote sensing data across the unique field laboratory of the East River, CO watershed, in collaboration with the Lawrence Berkeley Lab SFA. An inverse 1-D diffusion-reaction model constrained by soil $p$$CO_2$ and surface efflux rates was developed to calculate net CO_2 production rates (R_{CO2}) over time. Field measurements are accompanied by laboratory incubation experiments and a meta-analysis of literature studies to assess theoretical constructs needed to accurately capture the response of microbial respiration to variable soil moisture. In both field and laboratory studies, East River soil profiles demonstrate unique responses to precipitation events, and accurate prediction of the associated respiration of carbon requires a sophisticated modeling approach. To capture this behavior, we have built a ‘dormancy model’ which allows the native soil microbial population to respond transiently to the presence or absence of water. However, field measured R_{CO2} show a dampened respiration response to moisture delivery when plants are senesced, suggesting that vegetation status is also important control on soil respiration. Collectively, our results suggest that plant phenology regulates the response of soil respiration rates to pulse wetting events. In particular, these results emphasize the importance of the timing of snowmelt and the summer monsoon relative to phenology on soil CO_2 fluxes and their sensitivity to projected changes in climate.

Transport and Retention of Metal Reducing Motile Bacteria in Idealized Pore Geometries

Lazaro Perez[1], Rishi Parashar[1]*, Nicole Sund[1], Andy Plymale[2], Timothy Scheibe[2]

[1]Desert Research Institute, Reno, NV

[2]Pacific Northwest National Lab, Richland, WA

Contact: rishi@dri.edu

Project Lead Principal Investigator (PI): Rishi Parashar

BER Program: SBR

Project: University led EPSCoR Project

Project Abstract:

For several species of motile microorganisms, encompassing strictly anaerobic, facultatively anaerobic, and facultatively autotrophic bacteria, with capacities to reduce a range of metals and radionuclides, micromodel experiments were conducted in idealized pore networks under both flow and no-flow conditions. The micromodels were designed as chambers with small depth (10 µm and 20 µm) and properties of bacterial transport and retention (biofilm formation) were studied in the horizontal plane. The density of the bacterial solution was kept low to minimize the interaction between individual cells. Videos of bacterial motion were recorded at various magnifications and frequencies. Trajectories of individual cells ranging from several seconds to few minutes in duration were extracted in neutral conditions (in the absence of any chemical or redox gradient). Position of individual cells in the videos were found by filtering the difference in pixel intensity between the current video frame and the mean image over the duration of the video. Groups of pixels in the species size range were merged to estimate the location of the cell center. Locations of cell centers were connected to create motion paths, which were extracted by categorizing cells based on their previous speed. Cell trajectories that were collected from the videos were then analyzed to determinine the suitability of Fickian and non-Fickian transport models as a function of timescale and pore structure. Growth of biofilm in the micromodel was studied which includes determination of biofilm morphology and its relation to pore structure, and its effect on fluid properties such as porosity, velocity, and development of preferential channeling. The micromodel experiments and related model to study motile microorganisms' transport and retention is expected to provide pathway for development of methodologies to include upscaled bacterial motion properties in bioremediation implementations.

Influence of hyporheic exchange on coupled S-Fe-C biogeochemical cycling in riparian wetland sediments

Cara M. Santelli[1], Crystal Ng[1], Shreya Srivastava[1], Aubrey Dunshee[1], Daniel Kaplan[3], Kenneth Kemner[4], Maxim Boyanov[5]

[1]University of Minnesota, Minneapolis, MN
[2]Northwestern University, Evanston, IL
[3]Savannah River National Laboratory, Aiken, SC
[4]Argonne National Laboratory, Argonne, IL
[5]Bulgarian Academy of Sciences, Sofia, Bulgaria

contact: santelli@umn.edu

Project Lead Principal Investigator (PI): Cara Santelli

BER Program: SBR

Project: University Award

Riparian wetland hyporheic zones, where oxic surface water and anoxic groundwater mix, exhibit spatiotemporally dynamic conditions that drive steep redox gradients and promote hotspots of diverse and fluctuating microbial activity. Growing evidence suggests that highly active "cryptic" sulfur redox processes drive the fate of iron and carbon in riparian wetlands including the production of reactive intermediate S species that promote further biotic and abiotic redox reactions such as those coupled with Fe reduction and methane oxidation, thus supporting higher rates of sulfur biogeochemical cycling than otherwise expected in these low sulfate environments. As "cryptic" sulfur redox processes are not well constrained in freshwater systems, much uncertainty remains as to how these processes effect the fate of Fe and CH_4 and respond to dynamic hyporheic fluxes in natural field settings. The overall goal of this research is to develop a mechanistic understanding of coupled biotic-abiotic Fe-S-C cycles in hydrologically dynamic wetland sediments. One of our specific objectives is to evaluate the microbial community structure and potential function driving these cycles. 16S rRNA and fungal internal transcribed spacer (ITS) sequencing was used to investigate the microbial communities inhabiting 6 different sites in an organic-rich riparian wetland at Tims Branch, part of the Argonne Wetland Hydrobiogeochemistry SFA. Preliminary results reveal a diverse microbial community dominated by phyla Proteobacteria, Acidobacteriota, Chloroflexi and Actinobacteriota. Fungal communities were dominated by Ascomycota, Mortierellomycota and Basidiomycota in these sediments. Seasonal variations in geochemical and hydrologic conditions and sediment depth affected the relative abundance of these phyla. For example in wetland sediments under gaining stream conditions, aqueous iron increased at depth, the relative abundance of Crenarchaeota decreased substantially at those depths in both January and August. In January, sulfate concentrations in the wetland sediments decreased at the top 0-5 cm interval and then increased at greater depths, which was reflected in a decrease in the relative abundance of sulfate-reducing Desulfobacterota from shallower to deeper depths. Despite an opposite trend in sulfate concentrations in the wetland sediments in August as a result of hyporheic fluxes, an opposite trend was not observed for the relative abundance of Desulfobacterota suggesting a potential role of abiotic Fe-S cycling processes. These results indicate that hyporheic fluxes and fast redox processes impact microbial distribution. Further work, with respect to this objective will focus on correlating hydrological and geochemical parameters with microbial community structure and function to acquire a deeper understanding of the role microbes play in Fe-S-C cycles in these wetlands.

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

S. McKenzie Skiles*,[1] David Gochis,[2] Janice Brahney,[3]

[1]University of Utah, Salt Lake City, UT;
[2]National Center for Atmospheric Research, Boulder, CO;
[3]Utah State University, Logan, UT

Contact: m.skiles@geog.utah.edu

Project Lead Principal Investigator (PI): S. McKenzie Skiles

BER Program: SBR

Project: University Project

Project Abstract:

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

Computational Models of Dissolved Organic Matter

Jeremy C. Smith,[1,2*] Deepa Devarajan,[1,2] Scott C. Brooks,[2] Scott L. Painter,[2] Baohua Gu,[2] Jerry M. Parks[2], Liyuan Liang[1,2]

[1] University of Tennessee Knoxville, TN [2] Oak Ridge National Laboratory, Oak Ridge, TN Contact: (smithjc@ornl.gov)

Project Lead Principle Investigator (PI): Jeremy C. Smith

BER Program: SBR Project: University project

Dissolved organic matter (DOM) plays a significant role in the biogeochemical processes of the aquatic and terrestrial environments including the global carbon cycle, microbial metabolism, transport of nutrients and contaminants. DOM is a complex heterogeneous mixture of several organic units. Molecular level interactions between those component molecules are responsible for active roles of DOM. Therefore, it is important to understand the behavior of DOM at the atomistic/molecular level. Here, molecular dynamics (MD) simulations were used to explore the interactions between the component molecules of DOM. Model lipid, peptide, carbohydrate, lignin, and low molecular weight organic compounds were simulated along with cations in water for 200ns. Various components of DOM aggregate to form dynamic supramolecules consisting of a hydrophobic core and an amphiphilic exterior. The molecular surface of DOM is composed of both hydrophobic and hydrophilic groups allowing DOM to bind with polar and non-polar molecules. DOM models for Leonardite humic acid and Suwanee River DOM were constructed and validated based on their elemental compositions and other available properties. The DOM models will be used to estimate the physiochemical properties for the biogeochemical reactions of DOM. Further refinement of the DOM models will involve increasing the variety of building block molecules.

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

Martial Taillefert[1,*] (PI), Eryn Eitel[1], Thomas DiChristina[2] (co-PI), Hyun-Dong Shin[2], Frank Stewart[2] (co-PI), Anthony D. Bertagnolli[2], Nastassia V. Patin[2], Kenneth Kemner[3] (Co-PI), Scott Brooks[4] (Co-PI), Christa Pennacchio[5], and Stephen J. Callister[6]

[1]School of Earth and Atmospheric Sciences, Georgia Institute of Technology, Atlanta, GA 30332 [2]School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA 30332 [3]Biosciences Division, Argonne National Laboratory, Argonne, IL 60439

[4]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831

[5]Joint Genome Institute, Walnut Creek, CA 94598

[6]Environmental Molecular Science Laboratory, Richland, WA 99354

Contact: (mtaillef@eas.gatech.edu)

Project Lead Principal Investigator (PI): Martial Taillefert

BER Program: SBR

Project: University Project

Project Abstract: The dynamic of biogeochemical processes regulating nutrient and contaminant release in stream and wetland sediments and their role in carbon transformation cannot be predicted accurately by current reactive transport models (RTMs). These models largely rely on detectable changes in geochemical conditions to activate metabolic processes, are unable to accurately account for competition between microbial processes, and poorly constrain the effect of hydrological perturbations on biogeochemical processes. The objectives of this project are to: (i) develop new rate laws for RTMs that rely on a combination of high throughput omics (meta-genomic, -transcriptomic, -proteomic, -bolomic) and geochemical signatures to identify the underlying anaerobic microbial processes in stream and wetland sediments; (ii) describe the competition between the dominant metabolic processes involved in contaminant (U and Hg) mobilization; and (iii) more accurately quantify carbon transformation processes. A combination of meta-omic and geochemical signatures were used to identify the main anaerobic microbial processes in a Savannah River Site wetland (SRS) and Oak Ridge East Fork Poplar Creek (EFPC) sediment. Geochemical depth profiles suggested that Fe(III) reduction dominates carbon remineralization processes in SRS wetland sediments, whereas a combination of NO_3^- and Fe(III) reduction dominates EFPC sediments. Sediment slurry incubations designed to investigate the competition between anaerobic terminal electron accepting processes demonstrated that NO_3^- reduction was the fastest respiratory process and that Fe(III) reduction apparently became dominant once NO_3^- was depleted. Incubations also revealed that SO_4^{2-} reduction was inhibited by Fe(III) reduction and that this inhibition was enhanced by ferrihydrite addition. In turn, metagenomic signals were enriched in gene variants indicating that bacteria coupling anaerobic $\sum H_2S$ oxidation to NO_3^- reduction were dominant in EFPC sediments but not in SRS wetland sediments. Metagenomic data thus indicate that a cryptic sulfur cycle may be more significant than apparent by geochemical signals. The metagenomic data is currently being confirmed via complementary meta-transcriptomic and -proteomic analyses. A gene-centric kinetic model was developed that includes a set of new

rate laws to represent competition between microbial communities involved in carbon remineralization processes. The model calibrated with one set of incubations was able to reproduce all the incubation treatments, suggesting that it could be readily included in RTMs. Overall, this project demonstrates that: (i) a combination of high throughput omic and geochemical data is needed; and (ii) simple gene- centric models can be readily included in RTMs to accurately identify biogeochemical processes and the competition between microbial communities involved in contaminant transformation in sediments.

Decrease in Aqueous U(VI) Following an Influx of Oxidants into Organic-Rich Reduced Sediments

Karrie A. Weber[1,2], Jeffrey P. Westrop[1], Pooja Yadav[1], Vincent Noel[3], Arjen Van Veelen[3,4], John R. Bargar[3], Romy Chakraborty[5]

[1]University of Nebraska-Lincoln, Lincoln NE
[2]Daugherty Water for Food Institute, Lincoln, NE
[3]SLAC National Accelerator Center, Menlo Park, CA
[4]Los Alamos National Laboratory, Los Alamos, NM
[5]Lawrence Berkley National Laboratory, Berkley CA

Contact: kweber@unl.edu

Project Lead Principal Investigator (PI): Karrie A. Weber

BER Program: SBR

Project: University Project

Project Abstract: An existing paradigm describes that the influx of oxidants such as dissolved oxygen (DO) or nitrate will stimulate the oxidation of reduced chemical species such as iron, Fe(II), and uranium, U(IV). The change in redox state thus alters metal/radionuclide behavior and contributes to the generation of soluble and mobile U(VI) species influencing contaminant mobility. Field research results challenged the existing paradigm whereby low concentrations of an oxidant (DO) were directly amended into an alluvial aquifer and stimulated reducing conditions as well as a decrease in aqueous uranium concentrations (Rifle, CO; (Pan et al., 2018)). A series of laboratory experiments was initiated in batch reactors containing reduced, organic-rich, uranium bearing alluvial sediments (collected from Riverton, WY; SLAC SFA) test the impact of the influx of low oxidant concentrations (nitrate and DO) on uranium mobility. These reduced sediments were amended with anoxic bicarbonate buffered medium (Ar:CO_2, 80:20; pH 6.7) with and without the addition of an oxidant (nitrate or DO). Aqueous U concentrations decreased (KPA and ICP-MS) following the addition of the oxidant, nitrate or DO. No significant decrease in aqueous U(VI) concentrations were observed in unamended controls. XANES analysis revealed an increase in solid-associated U(VI) in DO amended reactors. However, the inverse was true in nitrate amended reactors. XANES analysis of sediments collected from nitrate amended reactors revealed an increase in the amount of U(IV) relative to the unamended controls (85% U(IV) in treatment relative to 31% U(IV) in control). In addition to observing the reduction of uranium, a significantly higher concentration of aqueous Fe(II) was also observed in treatments relative to an unamended control indicating active Fe(III) reduction. Concurrent with an increase in aqueous Fe(II), a decrease in sulphide was observed. While this result could be indicative of oxidation, PHREEQC modelling of geochemical data supports the precipitation of Fe-sulphide as a potential mechanism for sulfide loss. All geochemical changes were observed concurrent with an increase in cell and virus abundance indicating cell growth and microbial activity. No significant changes were observed in controls. Together these results indicate that U retention under oxidizing conditions may not be solely limited to solid-phase sequestration of U(VI) but also an influx of an oxidant such as nitrate that can stimulate U(VI) reduction leading to sequestration as U(IV). This challenges our current understanding of U mobility in natural systems and indicates overlooked controls governing U redox cycling.

Pan, D., Williams, K. H., Robbins, M., and Weber, K. A., 2018, Uranium Retention in a Bioreduced Region of an Alluvial Aquifer Induced by the Influx of Dissolved Oxygen Environ Sci Technol, v. 52, no. 15, p. 8133–8145.

Using Global Sensitivity Analysis to Identify Controlling Processes of Complex Systems

Ming Ye,[1,*] (Presenting Author), Li Li,[2] Xingyuan Chen,[3]

[1]Florida State University, Tallahassee, FL; [2]Pennsylvania State University, State College, PA; [3]Pacific Northwest National Laboratory, Richland, WA

Contact: Ming Ye(mye@fsu.edu)

BER Program: Subsurface Biogeochemical Research

Project: University-Led Research

Project Web: https://atmos.eoas.fsu.edu/~mye/DOE_ProcessIdentification.php

Project Abstract:

This project developed three new methods of global sensitivity analysis for identifying controlling processes of an environmental system that is always open and complex. For such a system, understanding all its processes and their interactions is difficult. On the other hand, since the system dynamics are determined mainly by controlling processes, efforts should be spent to better understand the controlling processes, and on the other hand, spending efforts on non- influential processes should be avoids. These are challenging because of uncertainty inherent in system processes. This project considers process model uncertainty (i.e., a process can be represented by more than one process model) and process parametric uncertainty (i.e., a process model parameter is not deterministically known but follows a distribution). The overarching scientific question to be answered in this project is as follows: *If we are not certain about the choice of process models and model parameters, can we correctly identify the controlling processes of a complex system?* We developed three methods of global sensitivity analysis to tackle this questions from different angles (theoretical and computational).

The first approach was developed for **process prioritization** to identify the process(es) that should be better understood to achieve the greatest reduction in the uncertainty of the output of system modeling. We developed a process sensitivity index, which is conceptually similar to the first-order sensitivity index of the Sobol' method. During this project, we developed a new computational method to substantially reduce the computational cost of calculating the process sensitivity index by reducing the computational cost from N^2 model runs to $2N$, where N is on the order of hundreds to thousands.

The second approach was developed for **process fixing** to screen non-influential process(es) with small contribution to the uncertainty of the output of system modeling. We developed a total process sensitivity index, which is conceptually similar to the total-effect sensitivity index of the Sobol' method. We evaluated this sensitivity index by using analytical functions and numerical groundwater models with three model uncertainty in the processes of land surface recharge, subsurface geology, and river boundary. This sensitivity index was also implemented using the computationally efficient method discussed above.

To further reduce the computational cost of process fixing, we developed the third approach that extends the design of Morris method for model parameters to model processes. Our methods reduces the number of model runs from thousands to tens, and the results are consistent with those of the total process sensitivity index discussed above,

Subsurface Biogeochemical Research

Federal Agency
SBR Science Focus Area

Active Groundwater Circulation and Permeability Observations Defined By Interdisciplinary Characterization of Geologic Controls in a Mineralized Headwater Catchment

Lyndsay Ball,[1*] Andrew Manning,[1] Richard Wanty,[1] Jeffrey Mauk,[1] Burke Minsley,[1] Bradley Carr,[2] Philip Verplanck,[1] Robert Charnock,[3] Beth Burton,[1]

[1] U.S. Geological Survey, Denver, CO; [2]University of Wyoming, Laramie, WY; [3]Colorado School of Mines, Golden, CO

Contact: (lbball@usgs.gov)

Project Lead Principal Investigator (PI): Richard Wanty/Burke Minsley

BER Program: SBR/Watershed Function SFA

Project: Characterization of groundwater flow and associated geochemical fluxes in mineralized and unmineralized bedrock in the upper East River and adjacent watersheds, Colorado

Project Website: https://minerals.usgs.gov/science/metal-transport-characterization- mineralized-mountain-watershed/index.html

Project Abstract: Geologic controls on groundwater flow, particularly in tectonically and topographically complex mountainous terrain, can be difficult to identify without a detailed understanding of subsurface geologic structure. This structure can influence the magnitude of groundwater flow at different depths within the mountain block, which in turn impacts the distribution and chemistry of groundwater discharge to the near-surface ecosystem.

Characteristic circulation depths and permeability structure in sedimentary-rock mountain blocks are particularly uncertain because the small number of studies that have determined the limits of circulation depth have been performed mainly in crystalline rocks, whereas sedimentary-rock sequences are typically more heterogeneous and anisotropic. We use a combination of geological, geophysical, geochemical, and hydraulic observations over multiple scales, including the detailed characterization of new high-elevation boreholes, to better understand the structure and hydrologic function of mountain bedrock aquifers. Our study focuses on the Redwell Basin in the Upper East River Watershed, CO, a high-elevation headwater catchment underlain by mineralized sedimentary rock. Long-interval depth-dependent packer tests indicate that substantial hydraulic conductivity ($K = 10^{-7}$ to 10^{-6} m/s) exists in the bedrock aquifer, and while permeability generally decreases with depth, some deeper intervals still exhibit relatively high K. In-situ observations from borehole geophysical measurements and drill core indicate the most hydrologically communicative features occur along sub-horizontal bedding plane fractures and at lithologic transitions, suggesting anisotropic permeability is inherited from the sedimentary structure and enhanced in the sub-horizontal direction. However, borehole temperature logs indicate a nearly linear thermal profile below a depth of 20 m with a gradient of 38ºC/km, indicative of low vertical groundwater flow velocities under a primarily conductive heat flow regime ($q < 1$ cm/yr). The chemistry of deeper groundwater (below 20 m) is substantially different from that of shallow groundwater: pH is 7-8 versus 4-5; specific conductance is 400- 600 versus 100-300 µS/cm; and concentrations of multiple constituents (e.g., Ca, Fe) differ by a factor >5. Tritium and He isotope data indicate that the deeper groundwater is dominantly >60 yr old, whereas shallow water is modern with apparent $^3H/^3He$ ages of 5-15 yr. The deeper water also has high terrigenic He concentrations of 4-8 times solubility, typical for groundwater 100's to 1000's of years old. Available temperature, chemistry, and age data therefore all suggest that, while

horizontal K may be high, vertical K is likely low, resulting in a relatively shallow active circulation depth of about 20 m.

Subsurface Biogeochemical Research

IDEAS-Watersheds Project

IDEAS-Watersheds: Accelerating watershed science through a community-driven software ecosystem

J. David Moulton[1*], Scott Painter[2], Sergi Molins[3], Xingyuan Chen[4], Reed M. Maxwell[5], Laura E. Condon[6], Steve Smith[7], Hai Ah Nam[1]

[1]Los Alamos National Laboratory, Los Alamos, NM, [2]Oak Ridge National Laboratory, Oak Ridge, TN [3]Lawrence Berkeley National Lab, Berkeley, CA, [4]Pacific Northwest National Laboratory, Richland, WA, [5]Colorado School of Mines, Golden, CO, [6]University of Arizona, Tucson, AZ,

[7]Lawrence Livermore National Laboratory, Livermore, CA

Contact: (moulton@lanl.gov) **BER Program**: SBR **Project**: IDEAS-Watersheds

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

Project Abstract:

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

In this poster we highlight the unique structure of the IDEAS-Watersheds project, which is organized around six Research Activities. There are three Partnership Activities, each undertaken jointly with one of SBR's interdisciplinary watershed focused SFA projects using concrete use cases to advance our watershed modeling capability. These projects include the Watershed Function SFA (LBNL - poster by S. Molins), the Critical Interfaces SFA (ORNL - poster by E. Coon), and the River Corridor SFA (PNNL - poster by X. Chen). A Continental United States (CONUS) Activity is advancing a basin-to-continental scale simulation platform (poster by L. Condon). A Reaction Network Activity partnering with SBR's fine-scale SFAs (ANL, LLNL, SLAC) focused on fundamental biogeochemical processes brings those advances into geochemistry reaction modeling tools. Finally, a Shared Infrastructure Activity coordinates the development of common workflow tools and software interfaces to support interoperability (see Workflows poster by S. Molins). To further leverage this structure to accelerate the development of watershed modeling capacity, we adopt a co-funding model with shared deliverables and joint funding of early career researchers. This approach creates a pool of IDEAS-SFA liaisons with most of their time focused on these shared deliverables, and hence, enables a variety of inter- SFA activities, such as our monthly training webinars in software development, and inter-SFA web-meetings exploring synergistic collaborations.

IDEAS-Watersheds: Partnership with the Watershed Function SFA

Sergi Molins,[1*], Ilhan Özgen-Xian[1], Zexuan Xu[1], Dipankar Dwivedi[1] , Daniil Svyatskiy[2], David Moulton[2], Carl Steefel[1]

[1]Lawrence Berkeley National Lab, Berkeley, CA, [2]Los Alamos National Laboratory, Los Alamos, NM

Contact: (smolins@lbl.gov)

BER Program: SBR

Project: IDEAS-Watersheds (LBNL)

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

Project Abstract: In this poster, we report progress on the two main IDEAS-Watersheds activities in support of the LBNL SFA Watershed Function Partnership. Specifically, we report on (1) the implementation of a general approach to generate multiresolution meshes for use in East River, CO, watershed simulations, and (2) the simulation of integrated-hydrology reactive transport processes in a hillslope and sub-catchment of the East River watershed. These activities combined set the stage for High Performance Computing (HPC) Scale-Aware simulations of flow and reactive transport at watershed scales in the second and third year of the project.

A wavelet-based local mesh refinement (wLMR) strategy was designed to generate multiresolution and unstructured triangular meshes from real digital elevation model (DEM) data, for efficient hydrological simulations at catchment-scale. The wLMR strategy was studied considering slope- and curvature-based refinement criteria derived from the DEM. Both criteria predicted outlet hydrographs with a close predictive accuracy to that on the uniform mesh, but the curvature-based criterion was found to slightly better the capture channeling patterns of real DEM data (Özgen-Xian et al, 2020, *Wavelet-based local mesh refinement for rainfall-runoff simulations*, Journal of Hydroinformatics, accepted March 2020)

Field observational data at the East River, CO watershed indicate that some aqueous geochemical components exhibit distinct characteristics under snowmelt and baseflow conditions. Geologic structure and mineral composition have a strong influence on the concentration-discharge (C-Q) response under different water infiltration and groundwater level scenarios. The Advanced Terrestrial Simulator (ATS) is used to simulate integrated surface- subsurface hydrology and reactive transport processes at an East River hillslope intensive site, and at the Copper Creek sub-catchment. The meteorological forcing combines the high- resolution PRISM precipitation reanalysis data, and the simulated evapotranspiration and snowpack from a land model. These simulations are used as a stepping stone in the use of the newly developed reactive transport capabilities of ATS, which were built upon the Alquimia interface and the concept of interoperable code development.

Unleashing Modeler Creativity: IDEAS on How Flexible Software can Further Process Understanding

Ethan T. Coon,[1]* Scott L. Painter,[1] Ahmad Jan,[1] and J. David Moulton[2]

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

Contact: (coonet@ornl.gov)

Project Lead Principle Investigator (PI): J. David Moulton

BER Program: SBR

Project: IDEAS-Watersheds. Los Alamos National Laboratory **Project Website**: https://ideas-productivity.org/ideas-watersheds/ **Project Abstract**:

Building process understanding through models requires a careful balance of process complexity and spatial scale. Too little process complexity or too coarse of a spatial scale insufficiently describes the system, while too much process complexity or too fine a spatial scale makes understanding difficult to glean from model runs. Finding this balance is central to the art of modeling and relies on the physical insights of the modeler. However, rigid software tools often make it difficult and time consuming to express these insights in models.

IDEAS-Watersheds, in building on work from IDEAS-Classic,[1] is exploring how an ecosystem of interoperable and flexible software tools can enable the fast construction of new models that are customized to a particular science question and informed by data. In partnership with the ORNL Critical Interfaces SFA, we show how mesh infrastructure, subgrid models, application programming interfaces, and flexible software design can come together to enable multiscale, multiphysics models of biogeochemical processing in stream corridors. Specifically, we represent transport in stream networks, and in each reach of the network, embed a travel-time based model of reactive transport to describe the processing of chemical components in streambeds and banks. The hierarchical structure of this model is enabled through Amanzi's infrastructure, while ATS's flow and transport processes are coupled to PFLOTRAN's geochemistry through the Alquimia interface. The resulting model allows biogeochemical processes to be represented at an appropriate spatial scale, while remaining computationally tractable compared to full 3D simulations. This type of model structural flexibility is a powerful tool for modelers, giving new insight into physical processes through investigations of model structure.

Coon, E.T., J.D. Moulton, and S.L. Painter. "Managing complexity in simulations of land surface and near-surface processes." *Environ. Modelling & Software* 78 (2016): 134-149.

IDEAS-Watersheds PNNL SFA Partnership: Multi-Scale River Corridor Hydrobiogeochemical Modeling

Xingyuan Chen[1,*], Hyun-Seob Song[2], Kewei Chen[1], Peishi Jiang[1], Joon Yong Lee[1], Chris Henry[3], Tim Scheibe[1], and David Moulton[4]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Nebraska-Lincoln, Lincoln, NE; [3]Argonne National Laboratory, Lemont, IL;

[3]Los Alamos National Laboratory, Los Alamos, NM;

Contact: (Xingyuan.Chen@pnnl.gov)

Project Lead Principle Investigator (PI): David Moulton

BER Program: SBR

Project: IDEAS-Watersheds

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

Project Abstract:

The IDEAS-Watersheds partnership with the PNNL SFA focuses on developing general workflows that leverage community software ecosystem to advance river corridor hydrobiogeochemical research, which will in turn be made available to the broader community. In the past year, we have developed an entire modeling pipeline from metagenomes to biogeochemical models and to reactive transport models, leveraging the DOE's KBase modeling platform. The core pipeline of the workflow include: 1) metabolic network construction from metagenomes; 2) identification of key substrates by metabolic pathway analysis; 3) development of stoichiometric and kinetic forms of biogeochemical reactions for the key substrates identified in the previous step, and 4) incorporation of the biogeochemical reaction model into a one- dimensional reactive transport model using PFLOTRAN. The workflow also allows optional steps that provide the methods for incorporating other omics datasets (such as metatranscripts, metaproteomics and metabolomics) when available. We have prototyped the workflow as KBase Apps using KBase Software Development Kit (SDK): one for translating chemical compositions from FTICR-MS into biogeochemical reaction models, and one for 1-D reactive transport modeling using PFLOTRAN. A KBase narrative using SFA example data has been made available to demonstrate the use of the Apps.

In collaboration with the National Center for Atmospheric Research (NCAR), we have also developed a data assimilation framework by linking Data Assimilation Research Testbed (DART) with PFLOTRAN. In addition to the access to various forms of ensemble data assimilation methods that are provided by DART, we have also implemented an ensemble smoother option that suits typical parameter estimation needs in SBR watershed research. We will further deploy DART-PFLOTRAN on KBase modeling platform as an App to facilitate assimilation of lab experimental data to estimate reaction kinetics parameters, thus enabling the ModEx iterations for batch- and column-scale biogeochemical predictive modeling. We have been working closely with other SBR SFAs to test the workflow design to broaden the science impacts.

IDEAS-Watersheds Continental Modeling Platform and Simulations

Laura E. Condon[*1], Reed M. Maxwell[*2], Steve Smith[3], Hoang Tran[2], Jun Zhang[1], Jen Steyaert[1], Adam Atchley[5], Dave Gochis[4], David Moulton[5]

[1]University of Arizona, Tucson, AZ , [2]Colorado School of Mines, Golden, CO, [3]Lawrence Livermore National Laboratory, Livermore, CA, [4]National Center for Atmospheric Research, Boulder, CO, [5]Los Alamos National Laboratory, Los Alamos, NM

Contacts: (lecondon@email.arizona.edu rmaxwell@mines.edu)

BER Program: SBR

Project: IDEAS-Watersheds (University)

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

Project Abstract: This project seeks to develop a high resolution, integrated hydrologic modeling platform for the Continental US (CONUS) that bridges across the IDEAS-watersheds study areas and provides a scaling framework from the reach scale up to watershed and regional systems. We are applying a phased approach to explore multiscale, multi-physics treatments of terrestrial hydrology modeling from the bedrock into the atmosphere. The continental research falls under three categories: (1) domain development, (2) software development and sustainability, and (3) simulations.

Domain Development - For the new CONUS domain we have been testing topographic smoothing and slope processing choices to improve runoff performance and simulations times. We have explored the impact of topographic parameterizations on watershed representation across spatial scales. We are also working on an improved subsurface representation combining multiple geologic datasets on, and developing reservoir operations datasets.

Software Development – This year we implemented two new overland flow boundary conditions in ParFlow. These were designed to improve performance by increasing consistency between surface and subsurface solution approaches, and to facilitate new model couplings by increasing the flexibility in boundaries.

Simulations – This year we published the warming simulations we completed on the first- generation domain. This study is a follow up to the simulations we did to quantify the impacts of human groundwater development. Combined these analyses allow us to compare top down and bottom up controls on groundwater surface water interactions. We have also been developing tools to subset and run watershed simulations from the CONUS domain. We demonstrated this with the Upper Colorado River Basin (UCRB) domain which was used to complete decadal simulations exploring the relationship between lateral groundwater flow and flooding.

IDEAS-Watersheds: Cross-cutting view and Integration– Workflows and Fine-scale activities

Sergi Molins[1], Xingyuan Chen[2], Kewei Chen[2], Scott Painter[3], Laura Condon[4,] Kate Maher[5], Tristan Babey[5], David Moulton[6]

[1]Lawrence Berkeley National Lab, Berkeley, CA, [1]Pacific Northwest National Laboratory, Richland, WA,

[3]Oak Ridge National Laboratory, Oak Ridge, TN, [4]University of Arizona, Tucson, AZ,

[5]Stanford University, Palo Alto, CA [5]Los Alamos National Laboratory, Los Alamos, NM

Contact: moulton@lanl.gov

BER Program: SBR

Project: IDEAS-Watersheds (LBNL)

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

Project Abstract: IDEAS-Watersheds is organized around six Research Activities driven by the Partnerships that the project has established with the different SBR SFAs and the CONUS simulation platform. However, it is in the sharing and contrasting of approaches between Partnership activities that the project meets the goal of advancing software development methodologies and engagement in the growing community-driven software ecosystem. In this poster, we provide a cross-cutting perspective of the IDEAS-Watersheds project along 3 themes that are used for project integration: geochemical modeling, workflows, and multi-scale approaches.

Geochemical modeling in IDEAS-Watersheds relies on PFLOTRAN and CrunchFlow. These codes are available as stand-alone codes as part of the software ecosystem but also as geochemical engines in other codes via the Alquimia interface. As part of IDEAS-Watersheds work, Alquimia has now been implemented in Parflow. We are also working on developing an Alquimia interface to PHREEQc. After this is complete, Amanzi-ATS and Parflow will be able to access either PFLOTRAN, CrunchFlow and PHREEQc.

The PNNL partnership has developed a new workflow that builds an entire modeling pipeline from metagenomes to biogeochemical models and to reactive transport models, leveraging the KBase modeling platform. The one-dimensional reactive transport component of the workflow has been tested on a column experiment in a natural reducing zone in collaboration with the SLAC SFA. The dataset is used to perform reactive transport benchmarking between PFLOTRAN, CrunchFlow and PHREEQC.

Different multiscale approaches are being developed for river-corridors that range from multi- resolution meshing to travel time-based approaches to represent exchanges between stream and the hyporheic zone. We contrast the workflows required to go from the river corridor data, to meshing the multiscale domains to performing the simulations. This is the first step towards an formal intercomparison between the different multiscale approaches.

Subsurface Biogeochemical Research

Argonne National Laboratory
SBR Science Focus Area

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

Kenneth Kemner[1]*, Pamela Weisenhorn[1], Maxim Boyanov[1,2] , Daniel Kaplan[3], John Seaman[3], Dien Li[3], Brian Powell[4], Angelique Lawrence[5], Christopher Henry[1], Ted Flynn[6], Man-Jae Kwon[7], Sen Yan[8], Yanxin Wang[8], Yamin Deng[8], Yiran Dong[8], Nancy Hess[9], Carlo Segre[10], Bhoopesh Mishra[11], Cara Santelli[12], Crystal Ng[12], Martial Taillefert[13], Jeff Catalano[14], Daniel Giammar[14], Christof Meile[15], Edward J. O'Loughlin[1]
[1]Argonne National Laboratory, Lemont, Illinois; [2]Bulgarian Academy of Science, Bulgaria; [3]Savannah River National Laboratory, Aiken, South Carolina; [4]Clemson University, Clemson, South Carolina; [5]Florida International University, Miami, Florida; [6]California Department of Water Resources, Sacramento, California; [7]Korea University, Seoul, Korea; [8]China University of Geosciences, Wuhan, China; [9]EMSL, Pacific Northwest National Laboratory, Richland, Washington; [10]Illinois Institute of Technology, Chicago, Illinois; [11]University of Leeds, Leeds, England; [12]University of Minnesota, Minneapolis, Minnesota; [13]Georgia Technical University, Atlanta, Georgia; [14]Washington University, St. Louis, Missouri; [15]University of Georgia, Athens, Georgia

Contact: (kemner@anl.gov)

Project Lead Principle Investigator (PI): Ken Kemner

BER Program: SBR

Project: Argonne Wetland Hydrobiogeochemistry SFA

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

Project Abstract: Within wetlands, movement of water and biogeochemically catalyzed transformations of its constituents determine the mobility of nutrients and contaminants, the emission of greenhouse gasses into the atmosphere, carbon (C) cycling, and the quality of water itself. The long-term objective of the Argonne *Wetland Hydrobiogeochemistry* Scientific Focus Area (SFA) is the *development of a mechanistic understanding and ability to model the coupled hydrological, geochemical, and biological processes controlling water quality in wetlands and the implications of these processes for watersheds commonly found in humid regions of the United States.* To accomplish this, the Argonne *Wetland Hydrobiogeochemistry* SFA studies hydrobiogeochemistry with a focus on a riparian wetland field site within Tims Branch at the Savannah River Site. This site is representative of many riparian wetlands found in humid regions of the Southeast that have C-rich soils and high Fe content. However, it is unique in that it received large amounts of contaminant metals and uranium as a result of previous industrial- scale manufacturing of nuclear fuel and target assemblies. Understanding the function of the wetlands in relation to water quality, including the concentration of metals and uranium within the soluble and particulate components of groundwater and surface waters of Tims Branch addresses the goal of the SBR Program to *advance a robust, predictive understanding of watershed function*.

The overarching hypothesis of our work is that *hydrologically driven biogeochemical processes that create redox dynamic conditions from the nanometer to meter scales are a major driver of groundwater and surface water quality within riparian wetland environments*.

We identified three major components of the Tims Branch riparian wetland that represent critical zones containing hydrologically driven biogeochemical drivers, which determine water quality: *sediment, rhizosphere, and stream*. These three components are interdependent and are considered as a whole for a systems-level

understanding to address our overarching hypothesis. Within these three focus areas, we identified two common thematic knowledge gaps that inhibit our ability to predict controls on water quality:

(1) In-depth understanding of the molecular-scale biogeochemical processes that affect Fe, C, and contaminant speciation within the wetland sediment, rhizosphere, and stream environments; and

(2) In-depth understanding of hydrologically driven biogeochemical controls on the mass transfer of Fe, C, and contaminants within wetland sediment, rhizosphere, and stream environments.

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

Coupled Iron and Uranium Biogeochemistry in Tims Branch, Savannah River Site

Edward O'Loughlin,[1*] Maxim Boyanov,[1,2] Daniel Kaplan,[3] Kent Orlandini,[1] 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;

Contact: (oloughlin@anl.gov)

Project Lead Principal Investigator (PI): Kemner BER Program: SBR

Project: Argonne Wetland Hydrobiogeochemistry SFA

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

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

Microtopographic controls on microbial community structure

Pamela Weisenhorn[1]*, Edward O'Loughlin,[1] Max Boyanov,[1,2] Tianhao Gu,[1] Daniel Kaplan,[3] Qizhi Zhang,[1] Christopher Henry,[1] Kenneth Kemner[1]

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

Contact: (pweisenhorn@anl.gov)

Project Lead Principal Investigator (PI): Kemner

BER Program: SBR

Project: Argonne Wetland Hydrobiogeochemistry SFA

Project Website: https://doesbr.org/documents/ANL_SFA_flyer.pdf

https://www.anl.gov/bio/project/subsurface-biogeochemical-research **Project Abstract**:

Wetlands are key features of watersheds that play an outsized role in affecting water quality because of their position within the landscape. The sharp and dynamic redox gradients typical of wetlands support a variety of microbial metabolisms and drive elemental transformations. Indeed, within wetland ecosystems even small changes in elevation can affect the local hydroperiod and alter the fate and transport of nutrients and contaminants. In this study, we examined the distribution of microbial taxa across microtopographic variation within the Tims Branch watershed on the Savannah River Site. Across the watershed, hydroperiod was an apparent driver of differences in microbial community composition. Microbial community composition aligned along this primary axis of variation, with lower elevation spots in the creek bed having the most dissimilar communities from higher elevation communities across all samples. Pit and mound microsites (formed when trees uproot) had distinct microbial communities, and these communities also varied by tree species. Further, local cm-scale heterogeneity in elevation at locations near the waterline resulted in differentiation of microbial community composition, with hummocks and hollows having consistently separable communities regardless of vegetation cover or position along Tims Branch. Considered together, these results suggest that fine scale variation in flooding regime and soil moisture can impact the structure of microbial communities and the functioning of watersheds.

We also examined the influence of contamination and disturbance (i.e. wild boar wallows) on microbial communities in this watershed. The effects of contamination and disturbance had a lesser effect. Microbial communities were mostly differentiated in response to disturbance, with communities that were different but overlapping in response to site contamination. While there were over 1,500 taxa that were unique to contaminated sites (of more than 20,000 taxa present in the communities from the contaminated sites), each of these taxa had low relative abundance. There was no effect of site contamination or disturbance on microbial diversity.

Biogeochemistry and Contaminant Speciation in Savannah River Site Sediments

Maxim Boyanov[1,2]*, Edward O'Loughlin,[1] Pamela Weisenhorn,[1] Daniel Kaplan,[3] Brian Powell,[4] Connor Parker,[4] Yanghao Shen,[5] Limin Zhang,[7] Hailiang Dong,[7,8] 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
[5]Lanzhou University, Lanzhou, Gansu, China
[6]Southwest University of Science and Technology, Sichuan, China
[7]China University of Geosciences, Beijing, China
[8]Miami University, Oxford, OH

Contact: (mboyanov@anl.gov)

Project Lead Principal Investigator (PI): Kemner

BER Program: SBR

Project: Argonne Wetland Hydrobiogeochemistry SFA

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

Project Abstract: The Argonne SBR SFA project (Wetland Hydrobiogeochemistry) focuses on the study of molecular to core-scale processes at a DOE field site, wetlands associated withTims Branch at the Savannah River Site. The site has characteristics typical of most riparian environments but is unique in that several contaminants (Ni, Cr, Zn, Pb, U) were discharged during past operations, providing an opportunity to study the effect of wetland processes on their long-term fate. Based on maps of the radiation distribution along Tims Branch, sediment cores were collected periodically at locations with elevated U concentrations. The in situ elemental distribution with depth was determined at 500-micron resolution by synchrotron x-ray fluorescence (XRF) spectroscopy on the intact cores, calibrated by acid digestion of subsamples. Results reveal that U is accumulated in the top 5-10 cm of the sediment at most locations, suggesting surface deposition and transport of contaminated particles. However, several locations showed U accumulation as deep as 25-30cm, suggesting porous media transport or burial. Correlations between some contaminants and mineral-specific elements (Fe, Ti) were observed. The in situ valence of U was determined using x-ray absorption spectroscopy (XANES) on the intact cores. Results show that in water-unsaturated sediments the predominant valence state is U(VI). In contrast, when U is present in water-saturated sediments the predominant valence state is U(IV), even within the 5-10cm layer that is close to the air-sediment interface. These results indicate a previously unappreciated importance of reduced U(IV) species controlling the mobility of U at this site. U L_{III}-edge EXAFS spectroscopy on sediment subsamples with high concentration of reduced U(IV) indicates that the reduced species is not mineralized uraninite (UO_2), but mononuclear U(IV) atoms associated with binding groups in the sediment. Comparisons to spectra obtained from defined mononuclear U(IV) species in laboratory reactors indicate that U(IV) in the sediment is not complexed to phosphate or carboxyl ligands, suggesting that U(IV) is not associated with organic material. The best spectral resemblance is to a mononuclear U(IV) species adsorbed on TiO_2, suggesting association of U(IV) with minerals in the sediment. Laboratory experiments indicate that Suwanee River humic acid is not able to complex U(IV) in co-precipitation experiments with U(IV). In contrast, the siderophore DFOB was found to complex U(IV) in the presence of reduced NAu-2 clay. The mechanistic understanding provided by these findings improve our ability to predict the transport of contaminants in natural environments using Reactive Transport Models.

Subsurface Biogeochemical Research

Lawrence Berkeley National Laboratory
SBR Science Focus Area

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

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

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]University of California, Berkeley CA; [3]Desert Research Institute, Reno NV; [4]Colorado School of Mines, Golden, CO; [5]Fort Lewis College, Durango, CO

Contact: sshubbard@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
Uncertainty associated with predicting watershed hydrobiogeochemical behavior remains high as climate change, extreme weather, wildfire, land-use change, and other disturbances significantly reshape interactions within the world's watersheds. The Watershed Function SFA is reducing this uncertainty through answering the grand challenge question: "how do mountainous watersheds retain and release water, nutrients, carbon, and metals?". The current phase focuses on how variability in snow accumulation and snowmelt timing and distribution influence mountainous watershed hydrobiogeochemical dynamics over sub-seasonal, seasonal and multi-annual timescales, with a focus on predicting aggregated water and nitrogen exports. The project is based within the East River Watershed, an emblematic mountainous headwater of the Upper Colorado River Basin, a region critical to U.S. water, energy and agricultural needs and one increasingly vulnerable to changing snow dynamics.

Given that mountainous watersheds embody significant gradients in vegetation, elevation, climate, and geology, their responses to disturbance are particularly complex, involving multi-physics, multi-scale processes occurring from bedrock through canopy, across land-water interfaces, and from genome-to-watershed scales. To confront this complexity, the Watershed Function SFA is developing new ways of conceptualizing, characterizing and predicting aggregated watershed system behavior. For example, the Watershed SFA takes a "system-of-systems" approach, where remotely sensed and ground-based information is used to develop a digital '4D East River Watershed', and machine learning approaches are used to identify key subsystems or "functional zones" within the watershed, which are hypothesized to have unique properties that influence the response to disturbance in that zone. Working within representative functional zones across the East River, process-based investigations paired with models are advancing predictive understanding of distributed hillslope ecohydrogeologic and river corridor responses to snow dynamics, the latter including processes occurring in the river, hyporheic zone, and across terrestrial-aquatic interfaces. A Scale-Adaptive Watershed Simulation Capability (SAWaSC) is being developed to enable 'telescoping' into regions that may have an outsized impact on larger watershed response to snow dynamics. SAWaSC will be compared with a functional zone approach for simulating aggregated watershed functional zone behavior using machine learning and hybrid modeling approaches. The functional zone approach to characterizing and modeling watershed system function is expected to provide a novel, site agnostic, and computationally efficient means for predicting aggregated system exports in response to perturbations that is scalable from catchment to drainage to basin scales.

Approaches to Identify and Predict Water Exports across and within Subsystems in the East River Watershed

Bhavna Arora[1*], Tetsu Tokunaga[1], Yuxin Wu[1], Rosemary Carroll[2], Jiancong Chen[3], John Christensen[1], Mark Conrad[1], Baptiste Dafflon[1], Amanda Henderson[4], Boris Faybishenko[1], Fadji Maina[1], Erica Siirila-Woodburn[1], Heidi Steltzer[4], Haruko Wainwright[1], Jiamin Wan[1], Chelsea Wilmer[4], Kenneth Williams[1] and Susan Hubbard[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]Desert Research Institute, Reno, NV; [3]University of California, Berkeley, CA; [4]Fort Lewis College, Durango, CO

Contact: barora@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
Understanding water partitioning as a function of perturbations is critically important for snow dominated mountainous systems, such as the East River watershed within the Upper Colorado River Basin. As such, a priority of the current phase of the Watershed SFA is to quantify and predict how snow dynamics, including snowmelt timing and variability in snowpack accumulation, affect water exports from hillslope to watershed scales. Within the East River watershed, significant uncertainty remains in association with evaluation of evapotranspiration (ET), groundwater recharge, and surface runoff, all of which vary significantly as a function of elevation, vegetation and topography. To improve the predictive understanding of water cycling and water exports associated with specific functional zones and in response to snow dynamics, we are: (a) constraining ET rates through measurements and models across scales and at sites located in functional zones having representative landscape characteristics, (b) collecting and synthesizing data on the impact of snow dynamics on water discharge, and (c) using high-resolution models to quantify hydrologic partitioning as a function of landscape position and snow dynamics. A key goal is to integrate field studies and associated observational datasets (e.g., stream discharge, LiDAR-derived snow water equivalent) into predictive models describing aggregated watershed hydrologic behavior.

For constraining ET rates, a Penman-Monteith model has been developed for four different locations covering meadow, conifer, and aspen within a lower montane functional zone referred to as the 'Pumphouse site'. ET partitioning is quantified using meteorological, energy, and water signals measured with a sensor suite that are further benchmarked through use of a mesoscale SMART soil experimental testbed. Further, existing field and remote sensing data are used to constrain predictive models like *ecosys* and ParFlow-CLM. In parallel, isotopic and geochemical data are used to provide constraints on estimates of groundwater recharge. In particular, seasonal variations in stable water isotopes of precipitation are used to apportion groundwater and runoff sources.

Given the complexity in snow melt and accumulation rates, ParFlow-CLM simulations are being used to assess the partitioning of water components in different functional zones and as a function of snow dynamics. The ParFlow-CLM model is being used to test the hypotheses that different functional zones have distinct water partitioning and residence times. These numerical investigations will inform the development and validation of functional zone-based models.

Exploring Climate and Bedrock Controls on Baseflow Age Distributions in a Snow- Dominated Mountainous Watershed

Rosemary Carroll,[1,*], Jeffrey Deems[2], Susan Hubbard[3], Andrew Manning[4], David Marchetti[5], Burke Minsley[4], Richard Niswonger[6], Sebastian Uhlemann[3], Craig Ulrich[3], Haruko Wainwright[3], Kenneth Williams[3], Erica Woodburn[3]

[1]Desert Research Institute, Reno, NV;
[2]National Snow and Ice Data Center, Boulder, CO; [3]Lawrence Berkeley National Laboratory, Berkeley, CA;
[4]U.S. Geological Survey, Denver, CO;
[5]Western Colorado University, Gunnison, CO;
[6]U.S. Geological Survey, Menlo Park, CA

Contact: rosemary.carroll@dri.edu
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
Groundwater contributions to streams, or baseflow, reflects the integrated effects of surface processes controlling groundwater recharge, the subsurface distribution of hydraulic conductivity, and the relative importance of groundwater circulating to different depths (different ages) for the generation of streamflow. Baseflow age reflects the time water spends in the subsurface interacting with host rock material to directly influence biogeochemical processes that control mineral weathering, including carbon and nitrogen dynamics. Identifying where and when climate affects recharge and groundwater flow paths are poorly understood in mountain basins, in part, due to a lack of observations characterizing snow distribution and subsurface hydraulic properties. We address data challenges by developing a framework for combining LiDAR Airborne Snow Observations (ASO) and novel methods for characterizing subsurface properties with a physically based hydrologic model. We demonstrate our approach in Copper Creek, CO (CC, 24 km^2), a snow-dominated, headwater catchment of the East River and embedded within the field testbed of the Lawrence Berkeley National Laboratory Watershed Function SFA. ASO provides confidence on the location and timing of water inputs to the basin, while high temporal observations of environmental gas tracers in stream water (N_2, Ar, SF_6 and CFC-113) indicate a minimum baseflow age of 10 years. To replicate the experimentally derived baseflow age with the hydrologic model requires an increase in bedrock permeability to partition more groundwater flow to deeper flow paths than originally simulated. Model results also indicate CC baseflow age is controlled by the ratio of recharge to hydraulic conductivity (R/K), with CC operating on a precipitation threshold defined by the historic median condition. Under historically dry conditions, recharge and water table elevations drop such that groundwater flow paths are less constrained by local topography, baseflow age becomes older and is increasingly sensitive to decreases in recharge. Looking forward, the model-experimental design is extended to the entire HUC10 East River (750 km^2). The increase in spatial extent will allow us to test the R/K conceptual model across landscape-scale gradients in snow accumulation, topography, vegetation and geology. ASO data will continue to constrain snowpack state, while ground and airborne geophysics are pursued to improve parameterization of lithology and geologic structure. Research stresses the need for alternative methods to characterize snow distribution and bedrock properties to link groundwater recharge and discharge zones, and quantify depth/age of groundwater flow paths and their propensity to shift toward longer timescales in a warming or drying climate.

The Resilience of Mountain Plants and their Role in Sustaining Ecosystem Services

Heidi Steltzer[1*], Amanda Henderson[2], Chelsea Wilmer[3], Dana Chadwick[4], Bhavna Arora[5], Nick Bouskill[5], Eoin Brodie[5], Rosemary Carroll[6], Jeff Deems[7], Baptiste Dafflon[5], Brian Enquist[8], Nicola Falco[5], Ben Gilbert[5], Carl Steefel[5], Erica Siirila-Woodburn[5], Tetsu Tokunaga[5], Charu Varadharajan[5], Haruko Wainwright[5], Yuxin Wu[5], Kenneth Williams[5], Susan Hubbard[5] and the Watershed Function SFA Team

[1]Fort Lewis College, Durango, CO;
[2]Rocky Mountain Biological Laboratory, Gothic, CO; [3]Colorado State University, Fort Collins, CO; [4]Stanford University, San Jose, CA;
[5]Lawrence Berkeley National Laboratory, Berkeley, CA;
[6]Desert Research Institute, Reno, NV;
[7]National Snow and Ice Data Center, Boulder, CO;
[8]University of Arizona, Tucson, AZ

Contact: steltzer_h@fortlewis.edu
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
Mountain plants are diverse, are evolved for stress and are unique from species in other ecoregions. As we dig deeper, literally and figuratively, into the traits and functions of mountain plants, the Berkeley Lab Watershed Function SFA is exploring hillslopes, river corridors, and elevational gradients to characterize the role of plants in mountain watershed function. Each new insight leads to further questions and redefining our thinking about mountain plants. Where we first began with a focus on the impact of drought conditions following earlier snowmelt, we've expanded to explore ways that many mountain plant species hold on to green leaves despite low soil water availability in surface soils, with some species maintaining growth and evapotranspiration even during dry times. Other species slow rates of growth and evapotranspiration, but do not senesce. Relatively few species brown down earlier, thus green cover may not reflect plant function. For mountain plants evolved for stressful conditions and short growing seasons, there are tremendous benefits to being ready to grow again as monsoon rains begin to fall. Using remotely sensed data from hillslope to watershed scales we are evaluating how to scale these observations and determine the Watershed Factors that influence plant species distributions and response. We are also comparing plot scale and remotely sensed observations with model predictions of 'monsoon rescue' of plant productivity following foresummer drought. The ability of mountain plants to withstand periodic drought prior to the onset of monsoons is an important example of their resilience to interannual variability in the hydrologic cycle and climate change. These responses are poorly understood but have major consequences for water partitioning, carbon and nutrient flux in these systems.

Landscape processes controlling nitrogen loss from mountainous systems.

Nick Bouskill[1,*], Michelle Newcomer[1], Taylor Maavara[2], Mark Conrad[1], Paula Matheus Carnevali[3], Jiamin Wan[1], Jill Banfield[1,3], Curtis Beutler[4], Markus Bill[1], Eoin Brodie[1], Wendy Brown[4], Rosemary Carroll[5], Wenming Dong[1], Nicola Falco[1], Patricia Fox[1], Ben Gilbert[1], Amanda Henderson[4], Reed Maxwell[6], Alex Newman[4], Peter Nico[1], Patrick Sorensen[1], Carl Steefel[1], Heidi Steltzer[7], Haruko Wainwright[1], Erica Woodburn[1], Susan S. Hubbard[1], Kenneth H Williams[1].

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]Yale University, New Haven, CT;
[3]University of California, Berkeley, Berkeley, CA; [4]Rocky Mountain Biological Laboratory, Gothic, CO;
[5]Desert Research Institute, Reno, NV;
[6]Colorado School of Mines, Golden, CO;
[7]Fort Lewis College, Durango, CO

Contact: njbouskill@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
Nitrogen is often a limiting element within mountainous ecosystems. Coarse soils, sparse vegetation, and strong hydrological events, such as snowmelt and monsoonal precipitation, can lead to significant losses of inorganic and organic nitrogen prior to assimilation and retention in plant and microbial biomass. Here we examine how rock weathering, atmospheric deposition, and biogeochemical cycling contribute to the aggregate signal of multiple years of nitrogen (nitrate, and DON) concentration-discharge data within contrasting pristine (East River) and metal- impacted (Coal Creek) catchments within the Upper Colorado River Basin. These paired catchments differ in terms of their bedrock properties and land cover. Coal Creek lithology is dominated by crystalline rock and sandstones, with conifers the predominant land cover type particularly on north-facing slopes. By contrast, a majority of the East River drainage is underlain by nitrogen-rich, marine black shale of the Mancos formation, with a mix of montane, subalpine, and alpine vegetation, with meadow species dominating. Both catchments are characterized by significant interannual variability in the CQ relationships for nitrate and DON, whereby chemostatic, and chemodynamic (both negative and positive) relationships are noted for both elements during different years. Despite higher export of nitrate from the predominantly shale- hosted East River, DIN: DON ratios suggest severe nitrogen limitation within both watersheds.

Intensive work within the East River has focused on two distinct spatial scales: (1) a hillslope-to- floodplain transect; (2) the entire 85km^2 drainage. By coupling long-term monitoring, field experiments, and mechanistic modeling we constrained a number of terrestrial fluxes for nitrogen including atmospheric deposition, nitrification, denitrification, and hydrological export. We note that shale weathering and atmospheric deposition are the dominant sources of nitrogen into the catchment. Furthermore, hydrological export represents only a small fraction of nitrate lost from the system, with denitrification likely responsible for the bulk of nitrogen loss. Furthermore, genomic data strongly suggests a high abundance of dissimilatory nitrate reduction to ammonium, representing a microbial ecosystem adapted towards minimizing loss by recycling nitrogen. We further note that within river nitrate export generally peaks during the peak discharge accompanying snowmelt, with minimum nitrate export occurring in the summertime. While this pattern likely represents the seasonal biological activity driving nitrogen retention during the growing season, more complex relationships are noted whereby nitrate exports do not scale linearly with discharge maxima. Overall, this work intends to improve understanding of the feedback between hydrological perturbation associated with snowpack dynamics and biogeochemical processes to improve predictions of nitrogen export at the watershed scale.

Hillslope factors that influence the mobilization and retention of nutrients and other elements

Eoin Brodie[1,2*], Bhavna Arora[1], Nick Bouskill[1], Sergio Carrero[1], Dana Chadwick[3], Mark Conrad[1], Chunwei Chou[1], Jill Banfield[1,2], Curtis Beutler[4], Markus Bill[1], Romy Chakraborty[1], Baptiste Dafflon, Brian Enquist[5], Sirine Fakra[1,8], Nicola Falco[1], Ben Gilbert[1], Zhao Hao[1], Amanda Henderson[4], Susan S. Hubbard[1], Ulas Karaoz[1], Alex Newman[4], Patrick Sorensen[1], Cole Sitar[1], Heidi Steltzer[6], Alex Thomas[2], Tetsu Tokunaga[1], Haruko Wainwright[1], Jiamin Wan[1], Shi Wang[1], Kenneth H Williams[1], Chelsea Wilmer[7], Xiaoqin Wu[1], Yuxin Wu[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA; [2]University of California, Berkeley, Berkeley, CA;
[3]Stanford University, Stanford, CA;
[4]Rocky Mountain Biological Laboratory, Gothic, CO;
[5]University of Arizona, Tuscon, AZ;
[6]Fort Lewis College, Durango, CO; [7]Colorado State University, Fort Collins, CO; [8]Advanced Light Source, Berkeley, CA

Contact: elbrodie@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
Hillslope processes critically regulate the rates at which nutrients become biologically available and the pathways and timescales over which water and elements solutes are transported to streams and rivers. Nutrient retention is enhanced through ecological soil-plant-microbe interactions and their synchronization with climate variables. In contrast, solute mobilization, including rock, mineral, and fluid biogeochemical reactions, generate flow paths and mobilize elements into the aqueous phase through the critical zone.

Our objectives are to (1) Determine how hydrological, soil-plant-microbe, mineral-fluid processes and their interactions influence water and element cycling at representative hillslope locations and their export to inland waters. By establishing mechanistic linkages between hillslope processes, our goal is to develop and evaluate predictive models that will be tested across a diversity of hillslope locations having unique characteristics. (2) Evaluate the sensitivity of export of elements to climate/disturbance from these locations as a function of dominant watershed factors that include geology, geomorphology, elevation, plant and microbial traits, and phenology characteristic of distinct watershed functional zones. (3) Develop sensor infrastructure to evaluate geomorphology and vegetation functional traits as windows into numerous subsurface properties. To date we: (1) have established a comprehensive integrated suite of weather, energy and soil sensors and deployed these at four locations at the East River lower montane site covering meadow, aspen and conifer areas; (2) are benchmarking these sensor suites using the prototype SMART Soils testbed; (3) have quantified inventories of bedrock elements, including nutrients and elements of water quality concern, and started to establish their pathways of release and impacts; (4) have identified slope and microtopographic controls on vegetation type and functional trait distribution that covary with subsurface physical properties at the hillslope scale, as well as covariance between vegetation functional types, soil chemistry and microbial metabolic potential; (5) have surveyed above- and below-ground plant traits at key moments in the water year that enable links between precipitation, ET, nutrient cycling to be understood mechanistically and linked to remote sensing methods; (6) have identified microbial metabolic potential for nutrient cycling across hillslope areas with different vegetation types; and (7) have started to connect hillslope-to-floodplain-to-river biogeochemical dynamics by developing zone-based transect models to quantify water and solute exports as a function of hydroclimate variance.

This information is used to challenge our understanding of how Watershed Functional Traits co- evolve at the hillslope scale such that remotely-sensed watershed-scale observables can be used to predict subsurface features relevant to elemental mobilization and retention.

River Corridor Redox Heterogeneity and Cycling: Impacts on Water Chemistry

Patricia Fox,[1] Michelle Newcomer,[1], Dipankar Dwivedi[1], Wenming Dong[1], Nick Bouskill[1], Markus Bill[1], Mark Conrad[1], John Christensen[1], Christian Dewey[2], Jillian Banfield[3], Paula B. Matheus Carnevali[3], Peter Nico[1]*

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]Stanford, Palo Alto, CA;
[3]University of California, Berkeley, Berkeley, CA

Contact: psnico@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
Herein we report an integrated field, lab, and modeling analysis of redox cycling along the river corridor of the East River drainage in Colorado. Particular attention is paid to the sulfur (S) cycle as being not only an important elemental cycle but also a good indicator and integrator of multiple redox processes. To understand biogeochemical potential of river corridor topsoils, we conducted metagenomic and metatranscriptomic investigations of microbial communities inhabiting three floodplains separated by >15km along the East River reach. Results have shown that the capacity for sulfide oxidation was found among the most abundant biogeochemical transformations, encoded in ~30–40% of the genomes detected across all three floodplains; capacities for thiosulfate or sulfite oxidation were found in < 20% of the genomes. Furthermore, transcription of genes encoding enzyme subunits involved in S transformations was found between the 50^{th} and 75^{th} percentile median range of transcription for all genes encoded in the genomes. These results suggest that sulfur transformations are a critical component of sulfur cycling in floodplains along the river corridor. In addition, analysis of meander sediments indicates a complex and redox variable array of S compounds supporting the idea of active S-cycling within the meanders. Modeling efforts have focused on understanding the functioning of individual meander features, as well as connected series of meanders and have been driven by synoptic sampling of river chemistry and Rn^{222} concentrations along two separate river reaches. As an example of single meander analysis, we quantified carbon (C) and S fluxes from representative high and low permeability sediments under seasonally transient hydrologic conditions. We assessed the sensitivity of these fluxes to (i) variable permeability distributions and (ii) changes in the timing and magnitude of hydrologic transients finding that C and S fluxes are greatest along flowpaths in high permeability sediments adjacent to low permeability zones. Further, we found that C and S fluxes increase as the duration and magnitude of peak river stage decreases and increases, respectively. To quantify subsurface geochemical exports along a full river reach, we carried out three-dimensional reactive flow and transport simulations for a 10-meander sub-system of the East River. Simulation results demonstrated that multi-directional exchanges were influenced by river stage, bathymetry, and meander geometry leading to both hot spot and hot moment controls on redox speciation. Results further demonstrate that scaling exponents typical for meanders are significantly different for oxidizing and reducing conditions.

Watershed Functional Zonation: Advancing Bedrock-to-Canopy Characterization across Watersheds

Haruko Wainwright[1], Nicola Falco[1], Sebastian Uhlemann[1], Qina Yang[1], Baptiste Dafflon[1], Burke Minsley[2], Jeff Deems[3], Craig Ulrich[1], Kenneth H. Williams[1], and Susan Hubbard[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA;
[2]U.S. Geological Survey, Denver, CO;
[3]National Snow and Ice Data Center, Boulder, CO

Contact: HMWainwright@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
Predictive understanding of watershed function and dynamics is often hindered by the heterogeneous and multiscale fabric of watersheds. In particular, ecohydrology and biogeochemical cycling involves complex hydrological-biogeochemical interactions occurring from bedrock-to-canopy, including geology, plants, microorganisms, organic matter, minerals and weathering products, dissolved solutes, and migrating fluids. Quantifying such interactions across heterogeneous watersheds is critical for estimating and predicting integrated hydrological and biogeochemical responses, such as carbon and nutrient exports, water resources and quality, as a function of both climate change and system disturbance. The Watershed Function SFA seeks to develop novel characterization methodologies to quantify complex watershed systems across scales, using advanced remote sensing, inversion, and machine learning approaches. We explore a variety of machine learning techniques – unsupervised learning, such as hierarchical and Bayesian clustering, and supervised learning, such as random forest – to gain a quantitative understanding of watershed organization and functionality. We hypothesize that (1) the co- evolution of terrestrial systems generates co-variability among subsurface/surface spatial features (e.g. topographic, plant, snow and geological metrics), (2) we can reduce the parameter dimensionality by exploiting such co-variability, and (3) we can identify several representative landscapes – so-called watershed functional zones – that capture distinct characteristics of those co-varied properties and associated watershed functions. We demonstrate our approach using airborne electromagnetic data, LiDAR-derived snow metrics, and hyperspectral data collected over the East River Watershed. Results show that unsupervised learning has the ability to resolve surface/subsurface co-variability, such as bedrock fracturing and plant species composition over the watershed, identifying several key zones that capture watershed-scale heterogeneity. Supervised clustering results indicate that elevation, aspect and geology are key controls on both drought sensitivity and nitrogen export, with the consequence being an ability to map watershed “functional” zonation and potentially prediction of annual nitrogen export in unmeasured sub-catchments given unique spatial features and peak snow water equivalent.

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

Characterization and Quantification of Plant Traits and Species at Watershed Scale: Analysis and Results from the NEON AOP Campaign at the East River watershed, Colorado

Nicola Falco[1*], Markus Bill[1], Ian Breckhiemer[2], Eoin Brodie[1], Philip Brodrick[4], K. Dana Chadwick[1,3], Jiancong Chen[1], Tristan Goulden[5], Kathleen Grant[3], Matt Hancher[6], Amanda Henderson[2], Aizah Khurram[1], Corey Lawrence[7], Katharine Maher[3], Maeve McCormick[3], John Musinsky[5], Samuel Pierce[8], Alexander Polussa[1], Maceo Hastings Porro[3], Andea Scott[3], Hans Wu Singh[9], Patrick Sorensen[1], Heidi Steltzer[10], Charuleka Varadharajan[1], Haruko Wainwright[1], Bizuayehu Whitney[1], C. F. Rick Williams[1], Kenneth H. Williams[1,2], Susan S. Hubbard[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA; [2]Rocky Mountain Biological Lab, Crested Butte, CO;
[3]Stanford University, Stanford, CA;
[4]Jet Propulsion Laboratory, Pasadena, CA; [5]National Ecological Observation Network; [6]Google Inc., Mountain View, CA;
[7]United States Geological Survey, Federal Center, CO;
[8]SLAC National Accelerator Laboratory, Menlo Park, CA;
[9]Scripps Institution of Oceanography, University of California San Diego, San Diego, CA;
[10]Fort Lewis College, Durango, CO

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

Project Abstract:
The Watershed Function Scientific Focus Area (WFSFA) aims to improve the predictive understanding of mountainous watershed hydrological and biogeochemical functioning, including the response to environmental perturbations. In such environments, plant communities play a critical role in hydrological and biogeochemical dynamics, given their principal role in the evapotranspiration and nutrient cycling. To capture such dynamics, it is necessary to accurately characterize the ecology governing such mountainous ecosystems.

To advance ecological characterization at the watershed scale, the WFSFA has acquired high- resolution visible-to-shortwave infrared hyperspectral and LiDAR data from airborne surveys over four headwater watersheds in the Upper Colorado Basin. The data were acquired by the NEON Airborne Observation Platform (AOP) during the summer 2018 via a collaborative proposal spanning multiple research institutions, including Lawrence Berkeley National Laboratory (LBNL), Rocky Mountain Biological Laboratory (RMBL), Stanford University, and UC Berkeley. The data acquisition was supported by a 3-week ground sampling campaign to collect foliage, litter, and soil samples along 14 hillslopes at various elevations and orientations. Data collection resulted in the characterization of 437 sites that encompass land cover dominated by trees, shrubs, and meadows. Other measurements included high-resolution RTK-GPS, near-surface geophysical measurements, soil moisture, and temperature.

Here we present cumulative results obtained from the analysis of the NEON data along with that derived from ground sampling. A first result is the estimation of plant species distribution across the entire study domain. We used machine-learning-based approach that integrated hyperspectral and LiDAR data to map plant species at 1-meter resolution. This spatial characterization allowed for further investigation of the coupling of plant distribution with topography and soil properties, revealing the strong impact of elevation on plant structure variability in tree species. Partial least squares regression was used to estimate plant traits, including foliar nitrogen concentration and leaf mass per area. Different models were built to estimate trait values for needle and non-needle leaf vegetation.

Ongoing research focuses on investigating the potential use of vegetation spectral signatures to provide insights on soil nutrient cycling and metal contaminants, the impact of bedrock type on forest traits, and quantification of water stress as pertains to tree mortality. This rich dataset will be integrated into Earth systems models to provide more accurate prediction of the future water resource and water quality in this region and along the Colorado River.

Linking River Corridor Processes and Watershed Zonation through Concentration- Discharge (C-Q) Analysis

Michelle Newcomer[1*], Nicholas Bouskill[1], Bhavna Arora[1], Tetsu Tokunaga[1], Jiamin Wan[1], Madison Burrus[1], Zexuan Xu[1], Maya Franklin[1], Haruko Wainwright[1], Dipankar Dwivedi[1], Fadji Maina[1], Erica Siirila-Woodburn[1], Rosemary Carroll[2], Peter Nico[1], Susan Hubbard[1]

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

Contact: mnewcomer@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
River corridor systems in snow-dominated, mountainous regions often express complex biogeochemistry and river water nutrient indicators as a function of watershed characteristics. River corridors host important subsystems for solute and nutrient processing at fine scales yet can have major impacts on large scale watershed exports as revealed by concentration-discharge (C-
Q) and export-discharge (E-Q) time series where export is defined as the mass flux of solutes. C- Q and E-Q statistical relationships can be built from surface, subsurface, and snowmelt compartments of the watershed. C-Q and E-Q statistical relationships offer critical insights into how watersheds respond to a range of snow scenarios and often display diagnostic patterns within a watershed network, such as clockwise or counter-clockwise hysteresis patterns. In this work we utilize daily C-Q and E-Q time series datasets, both measured and modeled, from our WFSFA 5- year time series of water quality and discharge data to capture interannual variability in climate conditions. Longer term historical USGS data is also used to analyze single-station and multi- station relationships across a range of watershed scales characterized by different watershed zones (i.e., patterns of watershed characteristics based on geology, vegetation). Efforts are underway to develop novel differential C-Q approaches that can characterize spatial variability in solute behavior, including methods to link watershed zonation patterns to C-Q and E-Q relationships. Additionally, we are utilizing a data-rich modeling approach with both subsurface, hyporheic, floodplain (i.e. MIN3P, PFLOTRAN) and large scale integrated hydrologic models (ParFlow- CLM) to investigate how river corridor subsystems, and large-scale hydrologic flow paths contribute to C-Q and E-Q relationships.

Results demonstrate significant differences in solute behavior within upstream versus downstream reaches. In particular, the heavily sinuous downstream section is marked by significant gains in both groundwater and solute concentrations, as opposed to the dilution and the declining trends observed in the higher-relief, fluvially energetic upstream reaches. Using numerical modeling, we demonstrate that during spring snowmelt, riverbed hyporheic zones support specific flow, biogeochemical, and microbial conditions that are more passive, leading to chemodynamic C-Q curves for nitrogen on the rising limb of the hydrograph. During the growing season, temperature, plants, microbes, and hydrologic gradients shift dramatically and lead to chemostatic C-Q behavior for nitrogen. Watershed zonation data revels strong controls of geology and vegetation on nitrogen exports. Our preliminary work indicates the importance of watershed features and development of zonation as a novel technique to understand C-Q.

Aggregated Watershed Modeling

Carl Steefel[1*], Dipankar Dwivedi[1], Sergi Molins[1], Erica Woodburn[1], Bhavna Arora[1], Fadji Maina[1], Zexuan Xu[1], Ilhan Ozgen[1]

[1]Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: cisteefel@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

Project Abstract:
We are pursuing several research directions to quantify water and biogeochemical cycling at the aggregated watershed scale using various modeling approaches. Within this modeling effort, so- called watershed Functional Zones play a key role insofar as they are the basis for various reduced order/dimension models for water and biogeochemical cycling. The elements of this research component include:

- *Zone-based transect modeling:* The functional zones that have been identified each represent a hillslope having distinct characteristics in both surface and subsurface features relative to neighboring parcels. For each intensive zone, we are creating a hillslope scale model (typically in 2D) and compare its response to early snowmelt relative to an average water year.
- *3D HPC modeling of surface+subsurface flow and biogeochemistry:* Using the software platform Amanzi-ATS, we are developing models for flow and biogeochemistry at the sub- catchment scale, initially focusing on the Lower Triangle. The HPC modeling makes use of adaptive mesh refinement to resolve smaller scale features (e.g., floodplains) that have an outsized impact on system behavior. This is one component of the Scale Aware Watershed Simulation Capability (SAWaSC).
- *Functional Zone refinement with HPC distributed computing:* High performance computing distributed modeling is being performed in select regions of the watershed to evaluate and refine the Functional Zone concept and to optimize the placement of sensor networks and other characterization data. A combination of ParFlow-CLM for hydrology and Amanzi-ATS for hydrology + biogeochemistry (both of which solve the for integrated surface-subsurface hydrology) are being used to determine whether various zones defined initially actually have similar functional responses as regards water and nitrogen export to various forcings and transients, especially as related to snow dynamics. Where this is not the case, the Functional Zones will be refined accordingly.
- *Reduced Order/Dimension SAWASC:* Building on insights from the HPC modeling task, a reduced-order (or semi-distributed) SAWaSC modeling approach is being developed to predict aggregated watershed discharge and nitrogen export as a function of snow dynamics. The approach is based on a residence time analysis within stretches of the river system, with lateral bedrock and hyporheic exchange taken from machine learning-based training on the high resolution distributed HPC sub-catchment simulations of biogeochemical cycling and fluxes and/or 1D stream tube reactive flow and transport simulations. The reduced order models will be further tested by synoptic sampling of stretches of the river system for discharge and concentration, with a focus on nitrogen. The zonation will be used to provide time-dependent lateral fluxes of water and biogeochemical species to the river system, i.e., C-Q relationships.

An End-End Pipeline for Watershed Data Management and Assimilation

Charuleka Varadharajan[1,*], Roelof Versteeg[2], Boris Faybishenko[1], Val Hendrix[1], Danielle Christianson[1], Dipankar Dwivedi[1], Matthew Henderson[1], Zarine Kakalia[1], Madison Burrus[1], and Deb Agarwal[1]

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

Contact: cvaradharajan@lbl.gov
Project Lead Principle Investigator (PI): Susan Hubbard
BER Program: SBR
Project: Berkeley Lab Watershed Function SFA
Project Website: watershed.lbl.gov

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

The Data Management Framework for the SFA provides infrastructure and services to support various aspects of the project's data lifecycle. The framework contains (a) a data collection and acquisition system involving a distributed sensor network across the watershed for diverse observations, (b) a queryable database with a workflow to telemeter and store data and associated data products with relevant metadata, (c) scripts for semi-automated QA/QC with cleaned data stored in the ERDB, (d) a data integration broker (BASIN-3D) to synthesize project data with external datasets for real-time queries, (e) an advanced data search and access portal for data discovery, exploratory analysis and download, and (f) periodic publication of data with DOIs in the DOE's ESS-DIVE repository.

These tools are used for building crosscutting data products needed for hypothesis testing and numerical modeling of hydrological and biogeochemical conditions in the East River watershed by both internal and external SFA project teams. The development and maintenance of this infrastructure presents a suite of challenges from practical field logistics to complex data processing that are addressed through various solutions. In particular, the SFA adopts a holistic view for data collection, assessment, and integration that dramatically improves the products generated, thereby enabling a co-design approach whereby data collection is informed by model results and vice-versa.

Subsurface Biogeochemical Research

Oak Ridge National Laboratory
SBR Science Focus Area

Biogeochemical transformations at critical interfaces in a mercury perturbed watershed scientific focus area

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

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[2]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830

Contact: (pierceem@ornl.gov)

Project Lead Principle Investigator (PI): Eric M. Pierce

BER Program: Subsurface Biogeochemical Research

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: Freshwater resources supplied by headwater streams and their surrounding watersheds are being threatened by severe pollution from anthropogenic releases of nutrients and trace metals (e.g., mercury [Hg]). Preserving these services for future use requires developing a deeper understanding of watershed structure and function. Research findings during Phase I of the Critical Interfaces Scientific Focus Area (SFA) project have led to the realization that transient storage zones (TSZs), and more specifically metabolically active transient storage zones (MATSZs), are hot spots for biogeochemical transformations that can exert a controlling influence on downstream water quality. TSZs are surface and subsurface locations (e.g., hyporheic zone) that delay the downstream flow of water in comparison to the main channel. In Phase II, the project aims ***to determine the fundamental mechanisms and environmental controls on Hg biogeochemical transformations in MATSZs in low-order streams***. A key component of this effort is to parameterize our biogeochemical modeling framework for predicting Hg transformations in East Fork Poplar Creek (EFPC).

In FY20, the SFA team has (1) added new capabilities to Advanced Terrestrial Simulator modeling software that integrates multiple components of EFPC watershed hydrology, (2) refined our transient availability model by including the impact sediment type has on net methylmercury (MeHg) production, (3) explored the transcriptional regulation of *hgcA* under different growth parameters, (4) examined complex biogeochemical controls on Hg methylation, and (5) performed assays of the HgcAB complex in a *E. coli* expression host and have taken significant steps to evaluate potential cellular metabolites essential for methylation activity. We have also explored the mechanisms of abiotic dimethylmercury formation using density functional theory (DFT) calculations and determined that Hg isotope exchange reactions can alter native mercury isotope compositions, complicating the interpretation of Hg methylation and demethylation assays. We developed a new approach that definitively determined the functional group assignments, electronic structure, and coordination geometry and binding interactions that characterize methanobactin-metal complexes and used this information to help explain the differences in Hg methylation potential caused by different types of methanobactin. Collectively, the aforementioned activities are providing a deeper understanding of Hg transformations in EFPC and allowing us to gain the process knowledge needed to improve predictions of Hg transformations at the scale of individual stream reaches and small watershed catchments.

Predicting Methylmercury Production Kinetics in Sediment with a Transient Availability Model

Grace E. Schwartz,[1] Regina L. Wilpiszeski,[2] Katherine A. Muller,[3] Scott Painter,[1] Dwayne Elias,[2] Scott C. Brooks[1]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[2]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[3]Earth Systems Science Division, Pacific Northwest National Laboratory, Richland, WA 99354

Contact: (schwartzge@ornl.gov)

Project Lead Principle Investigator (PI): Eric M. Pierce

BER Program: Subsurface Biogeochemical Research

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: East Fork Poplar Creek (EFPC) in Oak Ridge, TN, USA is contaminated with high concentrations of mercury (Hg). In the EFPC ecosystem, anaerobic microorganisms containing the *hgcAB* gene cluster transform Hg to monomethylmercury (MMHg), a neurotoxin that bioaccumulates in the food web. To improve understanding of watershed controls on Hg cycling, our research is designed to: (1) identify ecosystem compartments and hydro-biogeochemical conditions that govern net MMHg concentration, and (2) understand the extent to which groundwater–surface water exchange drives Hg transformations in EFPC. Our work develops a kinetic model for net MMHg production in EFPC sediment that accounts for competing processes that may reduce Hg availability for methylation and MMHg availability for demethylation. This transient availability model combines kinetic expressions for multisite sorption of Hg and MMHg, Hg(II) reduction/Hg(0) oxidation, and methylation/demethylation kinetics.

We conducted experiments in two EFPC sediment types: silty and sandy. The silty sediment has a longer water residence time and is relatively anoxic, carbon-rich, and more metabolically active compared to the sandy sediment. Despite these differences in sediment characteristics, sequencing of the *hgcAB*+ organisms in the two sediments revealed similar diversity distributions, with *Deltaproteobacteria* dominating. Microcosm experiments using stable Hg and MMHg isotopes were used to determine Hg and MMHg sorption rates to the sediments and to track methylation and demethylation in sediment slurry microcosms. We found a much higher MMHg production potential in the silty sediment compared to the sandy sediment. Demethylation rates were similar between the two sediments. Trends in Hg adsorption to the sediments were broadly similar, with moderately more and faster sorption to the silty sediment. MMHg sorption was very different between sediments with 85% of MMHg sorbing to the solid phase after 30h compared to only 24% in the sandy sediment.

Overall, results indicate that silty sediment would have greater overall MMHg production in EFPC due to the high MMHg production potential and long water residence time. However, in the sandy sediment, a large proportion of any MMHg that is produced could be readily delivered to the water column due to lower MMHg sorption rates. The similarity in methylator diversity in the sediments indicates that differences in MMHg production are not due to different methylating microbial communities but could be due to differences in *hgcAB*

expression or overall sediment productivity. Our results will be incorporated into a field scale model of EFPC to predict MMHg fluxes within the watershed.

Investigating the Dynamics of *hgcAB* and the Effect of Syntrophic Interactions on Hg-methylation

Caitlin Gionfriddo,[1] Regina Wilpiszeski,[1] Ally Soren,[3] Mircea Podar,[1] Josh Michener,[1] Brandy Barber,[1] Ann Wymore,[1] Grace Schwartz,[2] Scott Brooks,[2] Cynthia Gilmour,[3] Dwayne Elias[1]

[1] Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[2] Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[3] Smithsonian Environmental Research Center, Edgewater, MD 21037

Contact: (gionfriddocm@ornl.gov)

Project Lead Principle Investigator (PI): Eric M. Pierce

BER Program: Subsurface Biogeochemical Research

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: In the East Fork Poplar Creek (EFPC), anaerobic bacteria containing the *hgcAB* gene cluster, transform mercury (Hg) to monomethylmercury (MMHg). To improve our understanding of the MMHg generation potential, we are (1) determining the native function of *hgcAB* using genomics, biochemical pathway elucidation and fitness studies, (2) characterizing the EFPC microbial community, and (3) designing model microbial communities.

Identifying the native function of *hgcAB* is essential to predicting Hg methylation potential across a range of environmental systems. The possibilities include one-carbon metabolism for acetyl-CoA and methionine biosynthesis, metal resistance, or metalloid methylation. Here we explored *hgcA* expression patterns and regulation under different growth parameters using *Desulfovibrio desulfuricans* ND132. We utilized RT-qPCR and RNA-seq to observe changes in *hgcA* expression in conditions requiring postulated biochemical HgcAB functions (e.g. +/- formate, methionine, arsenate, mercury). Our results indicate that *hgcA* expression is significantly regulated across the growth stages under some conditions tested and may be regulated by *ars*R, typically known for regulating arsenate reduction and methylation genes. Deletion of *hgcAB* revealed differences in the transcriptome, proteome, metabolome, and metal speciation in growth media between wild-type and Δ*hgcAB* cultures as well as significant down-regulation of flagella and cilia, which has been confirmed by transmission electron microscopy. Significant differences in substrate consumption, acetate and biomass production, and expression of C1 metabolism proteins were observed between the strains under fermentative and sulfate- reducing conditions. The presence and abundance of Hg-methylators are often poor indicators for environmental MeHg concentrations. Therefore, understanding the molecular mechanisms of *hgcA* essential to expression and translation is needed to better predict environmental conditions that drive Hg-methylation potential in stream systems.

EFPC sediment and periphyton biofilm genomic analyses are the basis for designing model community experiments. Methylating and non-methylating species are being combined under the same geochemical conditions to determine whether the effect on Hg-methylation might be additive, subtractive or exponentially increased by complex multi-species interactions. We are actively monitoring for physiological changes (e.g., cell count, Hg-methylation rates, HgcAB expression levels) between experiment performed with single-species

versus co-cultures. The results are providing key details for unraveling measurements that are being performed with more complex EFPC natural communities in Theme 1.

Structural and mechanistic characterization of Hg transformations

Connor J. Cooper,[1,2] Kaiyuan Zheng,[3] Katherine W. Rush,[3] Alexander Johs,[2] Brian C. Sanders,[2] Georgios A. Pavlopoulos,[4] Nikos C. Kyrpides,[4] Mircea Podar,[1,2] Sergey Ovchinnikov,[5] Stephen W. Ragsdale,[3] Peng Lian,[1,2] Zhongyu Mou,[2] Scott C. Brooks,[2] Baohua Gu,[2] Niranjan Govind,[6] Sofi Jonsson,[7] and Jerry M. Parks[1,2,*]

[1] University of Tennessee, Knoxville, TN
[2] Oak Ridge National Laboratory, Oak Ridge, TN 37830
[3] University of Michigan Medical School, Ann Arbor, MI
[4] DOE Joint Genome Institute, Walnut Creek, CA
[5] Harvard University, Cambridge, MA
[6] Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99354
[7] Stockholm University, Stockholm, Sweden

Contact: (parksjm@ornl.gov)

Project Lead Principle Investigator (PI): Eric M. Pierce

BER Program: Subsurface Biogeochemical Research

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: Bacteria and archaea possessing the *hgcAB* gene pair methylate inorganic mercury (Hg) to form monomethylmercury (MMHg). HgcA consists of a corrinoid binding domain and a transmembrane domain, and HgcB is a ferredoxin. However, their detailed structure and function have not been thoroughly characterized. We modeled the HgcAB complex by combining metagenome sequence data, coevolution analysis, and ab initio structure calculations. In addition, we overexpressed HgcA and HgcB in *Escherichia coli* and confirmed spectroscopically that they bind cobalamin and [4Fe-4S] clusters, respectively, and incorporated these cofactors into the structural model. Surprisingly, the two domains of HgcA do not interact with each other, but HgcB forms extensive contacts with both domains. Conserved cysteine residues are likely involved in transferring Hg^{II} into position for methylation, removing methylmercury, or both.

Although anaerobic microorganisms are the primary producers of MMHg, the abiotic formation of dimethylmercury (DMHg) from MMHg has been suggested to account for a large portion of DMHg formation. Previous experimental work has shown that abiotic formation of DMHg from MMHg can be facilitated by reduced sulfur groups on mineral particles. Although a mechanism was proposed for this transformation, a more detailed investigation of this reaction is warranted. Thus, we performed density functional theory (DFT) calculations to explore mechanisms of DMHg formation on the surface of a nanoparticle model. We found that coordination of MMHg substituents to adjacent reduced sulfur groups protruding from the surface facilitates DMHg formation and that the reaction proceeds through direct transmethylation from one MMHg substituent to another. Coordination of Hg by multiple S atoms provides transition state stabilization and activates a C-Hg bond for methyl transfer. These findings provide insight into abiotic DMHg formation and fill gaps in our understanding of Hg transformation and cycling in the environment.

Biomolecular processes contributing to Hg transformations at critical interfaces

Xujun Liang,[1] Kaiyuan Zheng,[2] Swapneeta S. Date,[3] Jerry M. Parks,[1] Stephen W. Ragsdale,[2] Baohua Gu,[1] Alexander Johs[1,*]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[2]Department of Biological Chemistry, University of Michigan, Ann Arbor, MI 48109
[3]Department, Vanderbilt University, Nashville, TN 37235

Contact: (johsa@ornl.gov)

Project Lead Principle Investigator (PI): Eric M. Pierce

BER Program: Subsurface Biogeochemical Research

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: A complex, yet finite set of geochemical and biomolecular processes control mercury (Hg) transformations and net methylmercury (MeHg) production in the environment. A robust predictive understanding of Hg biogeochemistry requires knowledge about the underlying molecular mechanisms. The production of MeHg in anaerobic bacteria and archaea is mediated by the *hgcAB* gene cluster. Proteomics and immunoblot data suggest that the abundance of the proteins HgcA and HgcB in cells of the model Hg-methylating bacterium *Desulfovibrio desulfuricans* ND132 is extremely low. Thus, in order to characterize the function of HgcA and HgcB, we have coexpressed HgcAB in a *E. coli* expression host. Hg methylation assays with cell lysates demonstrate that the heterologously co-expressed HgcAB complex is able to convert added mercuric (Hg[II]) mercury to MeHg. In addition, to facilitate purification of the HgcAB complex for spectroscopic and structural characterization, we expressed a His_6-tagged HgcAB construct in *E. coli*, which also showed methylation activity in cell lysates. Interestingly, the methylation activity of all constructs is substantially enhanced after adding cell lysates from deletion mutants (Δ*hgcAB*) of *Desulfovibrio desulfuricans* ND132 and *Geobacter sulfurreducens* PCA suggesting that there are other cellular components contribute to the mercury methylation activity of HgcAB. Currently, we are evaluating cellular metabolites potentially involved in enhancing Hg methylation activity and have identified a positive correlation between the levels of exogenously added S-adenosyl methionine and Hg methylation rates. The present results establish the foundation for biochemical, spectroscopic and structural characterization of the HgcAB complex, which will provide essential information about the role of HgcA and HgcB in Hg(II) methylation and its integration with cellular metabolism.

Overlooked Mercury Isotope Exchange Reactions in Environmental Systems

Lijie Zhang,* Xia Lu, Xujun Liang, Eric M. Pierce, and Baohua Gu

Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830

Contact: (gub1@ornl.gov)

Project Lead Principle Investigator (PI): Eric M. Pierce

BER Program: Subsurface Biogeochemical Research

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: Enriched mercury (Hg) stable isotope tracers have been widely used in both laboratory and field investigations to assess biogeochemical transformations of Hg. However, previous studies rarely considered isotope exchange reactions between the newly added Hg isotope and the previously deposited Hg ("old"), as these reactions could result in redistributions of the new and "old" Hg isotopes in environmental matrices. This study examined isotope exchange kinetics of divalent Hg(II) species in various groundwater and soil matrices, including low-molecular-weight (LMW) thiols (e.g., cysteine and glutathione), dissolved organic matter (DOM), metacinnabar (β-HgS), and Hg-contaminated sediments. We found that Hg bound to LMW thiol ligands and DOM can be rapidly exchanged within minutes by the addition of another Hg isotope in a homogeneous solution. The exchange resulted in identical distributions of Hg isotopes when added at equal molar concentrations. Likewise, we observed rapid isotope exchange between newly added Hg and the mineral-associated "old" Hg(II), such as metacinnabar and a Hg(II)-contaminated sediment. However, isotope exchange did not occur between inorganic Hg(II) and methylmercury up to 2 days, likely due to the covalent bonding between Hg(II) and the methyl group. Together our results suggest potentially wide occurrences of isotope exchange reactions when an enriched Hg isotope is applied in environmental systems, and these reactions result in changes in isotopic compositions of Hg bound to organic or inorganic ligands and minerals. Therefore, interpretation of experiments using isotopically-enriched Hg without consideration of isotope exchange could lead to biased conclusions concerning Hg fate and transformation rates.

Spectroscopic Investigations of Late Transition Metal Complexes by Methanobactin Chromophores

Peter Eckert,[1,*] Alexander Johs,[1] Alan A. DiSpirito,[2] Jeremy D. Semrau,[3] Baohua Gu,[1] Eric M. Pierce[1]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[2]Roy J. Carver Department of Biochemistry, Iowa State University, Ames, IA 50011
[3]Department of Civil and Environmental Engineering, University of Michigan, Ann Arbor, MI 48109

Contact: (pierceem@ornl.gov)

Project Lead Principle Investigator (PI): Eric M. Pierce

BER Program: Subsurface Biogeochemical Research

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: Methanotrophic bacteria catalyze the aerobic oxidation of methane to methanol using enzymes with copper (Cu)-based active sites. To facilitate the acquisition of Cu ions some methanotrophic bacteria secrete small peptides known as methanobactins which strongly bind Cu and function as an extracellular Cu recruitment relay analogous to siderophores and iron. In addition to copper, methanobactins are known to form complexes with other late transition metals, including mercury (Hg). Methanobactins have a rich photochemistry and are ideal candidates for spectroscopic study, but a detailed characterization of their spectroscopic features remains incomplete and the solution-phase interactions of methanobactins with late transition metals remains ambiguous.

We present the first combined computational and experimental spectroscopy investigation of characterizing methanobactin-metal (i.e., zinc [Zn], Cu, and Hg) complexes. We observe characteristic differences in absorption spectra of methanobactin complexes with the three late transition metals and compare our experimental data with electronic structure calculations based on the coordination geometry observed in crystal structure data. Apart from characteristic absorbance changes, the complexation of methanobactin with transition metals results in a fluorescence emission. Drawing on previous investigations of the active site of the wild-type green fluorescent protein, we propose a mechanism for the observed fluorescence enhancement. We note spectroscopic indications of slow dynamical changes in mixtures of methanobactin-SB2 and Hg(II) and propose an Hg(II) -concentration-dependent oligomerization process. Collectively, our results shed new light on the binding interactions which characterize the chelation of late transition metals by methanobactin peptides.

Synergistic effects of a chalkophore, methanobactin, on microbial methylation of mercury

Baohua Gu,[1,*] Lijie Zhang,[1] Xixiang Yin,[1] Lihong Wang,[1] Xujun Liang,[1] Alan A. DiSpirito,[2] Jeremy D. Semrau[3]

[1]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830
[2]Roy J. Carver Department of Biochemistry, Iowa State University, Ames, IA 50011
[3]Department of Civil and Environmental Engineering, University of Michigan, Ann Arbor, MI 48109

Contact: (gub1@ornl.gov)

Project Lead Principle Investigator (PI): Eric M. Pierce

BER Program: Subsurface Biogeochemical Research

Project: Oak Ridge National Laboratory Critical Interfaces Scientific Focus Area

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

Project Abstract: Microbial production of the neurotoxin, methylmercury (MeHg), is a significant health and environmental concern as it can bioaccumulate and biomagnify in the food web. While the genetic basis of microbial mercury methylation is known, factors that control net methylmercury (MeHg) production in the environment are still poorly understood. A chalkophore or a copper-binding compound, termed methanobactin (MB), has been shown to form strong complexes with mercury [as Hg(II)] and also enables some methanotrophs to degrade MeHg. It is unknown, however, if Hg(II) binding with MB can also impede Hg(II) methylation by other microbes. Contrary to expectations, MB produced by the methanotroph *Methylosinus trichosporium* OB3b (OB3b-MB) enhanced the rate and efficiency of Hg(II) methylation more than that observed with thiol compounds (such as cysteine) by the mercury-methylating bacteria, *D. desulfuricans* ND132 and *G. sulfurreducens* PCA. Compared to no-MB controls, OB3b-MB decreased the rates of Hg(II) sorption and internalization, but increased methylation by 5–7 fold, suggesting that Hg(II) complexation with OB3b-MB facilitated exchange and internal transfer of Hg(II) to the HgcAB proteins required for methylation. Conversely, addition of excess amounts of OB3b-MB or a different form of MB from *Methylocystis* strain SB2 (SB2-MB) inhibited Hg(II) methylation, likely due to greater binding of Hg(II). Collectively our results underscore complex roles of exogenous metal-scavenging compounds produced by microbes and their interactions with others in controlling net production and bioaccumulation of MeHg in the environment.

Subsurface Biogeochemical Research

Pacific Northwest National Laboratory
SBR Science Focus Area

River Corridor Hydrobiogeochemistry from Reaction to Basin Scale

Tim Scheibe[1*], Xingyuan Chen[1], Emily Graham[1], James Stegen[1], and the PNNL SBR SFA Team

[1]Pacific Northwest National Laboratory, Richland, WA

Contact: (tim.scheibe@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov

The Pacific Northwest National Laboratory (PNNL) Subsurface Biogeochemical Research (SBR) Science Focus Area (SFA) will transform understanding of spatial and temporal dynamics of coupled hydrologic and biogeochemical processes in river corridors (hydrobiogeochemical function) from reaction to watershed and basin scales, thus enabling mechanistic representation of river corridor processes and their response to disturbances in multiscale models. Rivers serve as integrators of watershed processes as their composition and dynamics reflect the conditions of the surrounding landscapes and subsurface environments. Hydrologic exchange flows (HEFs) between river channels and surrounding sediments are a ubiquitous feature of river corridors but vary substantially in their character and impacts. HEFs and the biogeochemical activities they promote are a critical component of river corridor hydrobiogeochemical function, yet we lack transferable understanding of how governing processes vary through space, time, and across scales. Furthermore, the representation of river corridors in basin-scale integrated land surface models is currently limited, and their cumulative impacts on watershed function are poorly understood. Accordingly, it is difficult to predict how river corridor hydrobiogeochemistry will respond to future disturbances. Our team is developing mechanistic understanding of the processes that link hydrologic, geochemical, and microbial processes in river corridors and integrating that new knowledge into numerical models at scales from fundamental reactions to major river basins to enable robust prediction. Wildfires and modified precipitation regimes are key disturbances that influence river corridor hydrobiogeochemistry and are prevalent in the Columbia River Basin (CRB). To elucidate the impacts of these disturbances, and working toward the vision stated above, we will expand our scope to span the CRB and, in collaboration with other SBR SFAs, other major basins across the contiguous United States. We will use a distributed, open science approach based on our successful development of WHONDRS to develop regional and national partnerships that will underpin this research. A multiscale ModEx approach will integrate process-based and data-driven models with experiments and observations across reaction to basin scales in coupled iterative learning cycles. Connecting project outcomes to the efforts of other agencies will ultimately enable robust watershed predictions to facilitate the solution of national challenges in water quality/quantity and Earth System prediction.

Quantifying Cumulative Effects of Coupled Organic Matter and Nitrogen Cycling in River Corridors across the Columbia River Basin

Kyongho Son[1*], Yilin Fang[1], Jesus Gomez-Velez[2], Pin Shuai[1], Heping Liu[3], Kevin Bladon[4], James Stegen[1], Emily Graham[1], Glenn Hammond[5] , Tim Scheibe[1], and Xingyuan Chen[1]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]Vanderbilt University, Nashville, TN; [3]Washington State University, Pullman, WA; [4]Oregon State University, Corvallis, OR; [5]Sandia National Laboratories, Albuquerque, NM

Contact: (Kyongho.Son@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to quantify the cumulative effects of river corridor hydrologic exchange flows (HEFs), dissolved organic matter (DOM) chemistry, and microbial activity on biogeochemical cycling, water quality, and contaminant mobility across the Columbia River Basin (CRB) under both baseline and disturbance conditions. River corridors play important roles in organic matter and nitrogen cycling and removal of excess nutrients. At basin scales, the incorporation of hydrologic connectivity and molecular information on microbiome structure (i.e., species composition and distribution of enzyme-encoding genes), microbial expression, and metabolomes will greatly improve a river corridor model (RCM) in capturing distinct water quality signatures in connection to variations in land use, hydrogeology, climate, and disturbances.

We have developed a multi-rate mass transfer (MRMT) RCM, SWAT-MRMT-R, to account for biogeochemical effects of HEFs within river corridors, resolving reactions that occur in both the surface water column and the hyporheic zones. Applying this RCM along the Hanford Reach has led to the new understanding that (1) traditional transient storage model that uses a single exchange coefficient overestimates denitrification in river corridors compared to MRMT; and (2) the locations of NO_3^- entering the river has a significant impact on nitrate retention and reduction due to spatial variability of HEFs.

We will enhance the mechanistic foundation of the RCM by linking dynamic river flow processes and heterogeneous terrestrial inputs with variable temperatures and reaction kinetics informed by molecular properties to investigate water, energy, and solute fluxes between the river-groundwater interface. Our RCM will provide the flexibility to leverage distributed molecular data from WHONDRS. We will tightly integrate modeling with experiments to advance the predictive understanding of the river corridor biogeochemistry; Initial model outputs will be used to focus field and laboratory experiments on biogeochemical hot spots and hot moments, which will then be used to refine mechanistic process representations (e.g., reaction network and kinetics) and parameterizations of RCM. The new RCM will enable the basin-scale predictions of cumulative effects of biogeochemical reactions influenced by HEFs, DOM chemistry and microbes, and will significantly improve the current state-of-the-art model that only estimates the reaction potentials. It will allow us to address questions like which watershed characteristics control spatial/temporal variations in river corridor biogeochemistry and how river corridors mediate watershed responses to disturbances. Beyond CRB, our approach can be generalized and applied to other basins facing environmental disturbances and water challenges with national significance.

Quantifying Basin-Scale Hydrological, Biogeochemical and Thermal Inputs to River Corridors Under Baseline and Disturbance Conditions

Xingyuan Chen[1*], Pin Shuai[1], Kyongho Son[1], Glenn Hammond[2] , Gautam Bisht[1], Heping Liu[3], Peishi Jiang[1], Kyuhyun Byun[1], Kevin Bladon[4], Yilin Fang[1], Xuehang Song[1], James Stegen[1], and Emily Graham[1]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]Sandia National Laboratories; Albuquerque, NM; [3]Washington State University; Pullman, WA; [4]Oregon State University, Corvallis, OR

Contact: (xingyuan.chen@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to provide spatially and temporally distributed inputs of water, solutes, and energy to river corridors under baseline and disturbed conditions using integrated watershed models. Disturbance by wildfires, in combination with post-fire precipitation scenarios, can dramatically influence dominant surface and subsurface flow paths and residence times, as well as water, energy, and dissolved organic matter (DOM) inputs to river corridors. However, the impacts of such disturbances on water quantity and quality remain poorly understood. Our previous studies have shown that river corridor processes are strongly influenced by hydrological, biogeochemical, and thermal inputs from the surrounding surface and subsurface environments. Integrated watershed models can link potential controlling factors (e.g., precipitation distribution, surface and subsurface flow paths, land use and disturbance histories) to define the heterogeneity and dynamics of these inputs that drive river corridor biogeochemistry, allowing more accurate evaluation of the roles of river corridors in mitigating or enhancing watershed responses to environmental disturbances.

We will develop and improve integrated hydrologic and biogeochemical watershed models using community codes hosted in the model ecosystem of IDEAS-Watersheds, linking hydrologic and biogeochemical models through particle tracking, tracer simulations, and interfaces to available biogeochemistry engines. We will use a paired-watershed (disturbed vs. reference) approach under various climate scenarios to evaluate the impacts of wildfires and precipitation on watershed functions. To incorporate wildfire impacts into watershed models, we will relate soil burn severity maps to key factors that control surface and subsurface flow and transport pathways. We will leverage available eddy covariance flux tower network data to better understand and quantify how wildfires change ecosystem structure and functions, modify soil properties, and alter land surface processes including surface energy budget components, and CO_2 fluxes at multiple spatiotemporal scales. These data will inform the parameterization of ecohydrological components of our watershed models under environmental disturbances.

Integrated watershed models are fundamental to understanding terrestrial inputs to river corridors under baseline and disturbance conditions. Our model will enable the evaluation of the interplay between hydrologic connectivity and terrestrial DOM (including pyrogenic organic matter) transport to rivers through both surface and subsurface pathways, thus enabling mapping of hydrobiogeochemical regimes across watersheds and basins without the need to measure everything and everywhere. Stream and riverbed temperature regimes simulated by the model can also be used to map thermal refugia for resilient aquatic habitat.

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

Matt Kaufman[1*], Bob Hall[2], Jesus Gomez-Velez[3], and James Stegen[1]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Montana, Polson, MT; [3]Vanderbilt University, Nashville, TN

Contact: (matthew.kaufman@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to 1) identify places/times across the Columbia River Basin (CRB) in which sediment-associated metabolism strongly influences active channel biogeochemistry, and 2) reveal drivers of underlying molecular properties. Sediment-associated organisms contribute from 3-96% of river corridor respiration. To represent these processes in predictive models, understanding how and why they vary in space and time is critical. Our team's recent work predicts spatial variation in sediment contributions to respiration (ERsed). To evaluate these predictions, we will use dissolved oxygen (DO) sensors across 1st-8th order streams in the Columbia River Basin (CRB). Sites will be in 4 sub-basins. At each location we will deploy two DO sensors: one open to channel water and one in a transiently open/closed chamber for 'dark bottle' incubations (DBIs). Results will be modeled to estimate total respiration for the integrated system (ERtot). Gross primary production (GPP) will be modeled by combining the DO data with stream morphology and flow. DBIs will be used to estimate respiration in the water column (ERwater). ERsed is found by difference: ERsed=ERtot- ERwater. Repeated DBIs will estimate dynamics of ERsed, which has never been quantified at the basin scale. Outcomes will be compared to NEXSS model predictions to guide additional mechanistic representation), enabling basin-scale ModEx.

At locations with large ERsed, we will study dissolved organic matter (DOM) chemistry and microbial gene expression. Field surveys across scales (expanded significantly by WHONDRS) indicate a diverse and variable molecular composition of DOM. Given the high reactivity of channel sediments, we expect DOM chemistry in both surface and pore waters will vary across reaches with large ERsed. Furthermore, microbes are key to translating variation in DOM chemistry to shifts in biogeochemical rates and solute dynamics. In turn, we expect reach-scale gradients in DOM chemistry, microbial gene expression, and nutrient concentrations. We will use surface water, pore water, and sediment samples distributed across reaches with large ERsed to test these hypotheses. DOM chemistry will be characterized using FTICR-MS, GC-MS, LC- MS, and NMR. Microbial gene expression will be quantified via metatranscriptomics, leveraging our active JGI project building a database of river corridor microbial genomes across >400 sites.

Biogeochemical Consequences of DOM Chemistry, Microbial Gene Expression, and Nutrient Concentrations: Integration between Lab Experiments and Substrate/Microbially-Explicit Models Linked to Reactive Transport

Hyun Song[1*], Jianqiu Zheng[2], Vanessa Garayburu-Caruso[2], Emily Graham[2], Matt Kaufman[2], Kelly Wrighton[3], and James Stegen[2]

[1]University of Nebraska-Lincoln, Lincoln, NE; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Colorado State University, Fort Collins, CO

Contact: (hsong5@unl.edu)

Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to understand biogeochemical consequences of variation in DOM chemistry, microbial gene expression, and nutrient concentrations, and integrate that knowledge with a modeling framework that couples these features with reaction network and reactive transport models. Here we will experimentally evaluate the biogeochemical consequences of variation in DOM chemistry, microbial gene expression, and nutrient concentrations. We will extend analyses beyond net respiration rates to data/insights needed for reaction network models that couple DOM with nutrient cycles. Previously the SFA has used high resolution DOM characterization, nutrient concentrations, and respiration rates to reveal that aerobic respiration undergoes a metabolic paradigm shift from DOM thermodynamic regulation under C-limitation to N-mining regulation under C-replete environments. The functional forms and cross-system generality of such relationships remain unknown, however.

These knowledge gaps limit our ability to represent basin-scale spatial and temporal changes in mechanisms linking DOM chemistry, microbial gene expression, and nutrient concentrations to river corridor hydrobiogeochemical function.

We will use a combination of laboratory experiments (batch reactors) and reaction network modeling to resolve knowledge gaps and provide a process-based modeling framework. Lab experiments will use sediments from reaches with maximum contributions from sediment to river corridor respiration in each of four sub-basins across the Columbia River Basin (CRB).

Sites will span CRB functional zones to evaluate transferability of experimental outcomes and associated models. DOM concentration and the presence of organic N will be manipulated, followed by measurements of respiration, nutrients (e.g., NH_4^+, NO_3^-, Fe(II), N_2O), DOM molecular properties (FTICR-MS, GC-MS, LC-MS, NMR), and microbial metatranscriptomes.

Data spanning DOM chemistry, gene expression, and nutrient concentrations will be used with a cheminformatics/metabolic modeling pipeline linking molecular information to 1D PFLOTRAN in KBase. A critical component is leveraging multi-omic data to identify biogeochemical reaction networks for reactive transport modeling in PFLOTRAN. Models will be run independently in each sampled field location. Simulated dynamics of DOM chemistry, gene expression, and solute transformations will be studied using machine learning and other data-driven modeling techniques to discover simplified representations of the linkages among molecular properties/processes and nutrient dynamics across environmental conditions. This will provide a foundation for reduced-order basin-scale models that link molecular properties/processes to basin-scale hydrobiogeochemical dynamics.

Temporal Trajectories of Wildfire Effects and their Relationship to Precipitation in the Columbia River Basin

Bob Danczak[1*], Allison Myers-Pigg[1,2], Kevin Bladon[3], Vanessa Garayburu-Caruso[1], James Stegen[1], and Emily Graham[1,4]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]Marine Sciences Laboratory, Pacific Northwest National Laboratory, Sequim, WA; [3]Oregon State University, Corvallis, OR; [4]Washington State University, Richland, WA;

Contact: (robert.danczak@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to understand trajectories of wildfire effects on river corridors and their relationship to precipitation. It will also provide a foundation for understanding relationships between wildfires and river corridor biogeochemistry across watershed features. Wildfires impact rivers across timescales due to variation in precipitation, evapotranspiration, soil hydraulic properties, and pyrogenic inputs. Further, our previous work illustrates that compounding wildfire and precipitation events can drive distinct changes in soil carbon and nitrogen cycles relative to a single event, putatively altering river corridor impacts. Thus, there is a need to understand trajectories of wildfire impacts (e.g., across gradients of time- since-fire) on river corridor biogeochemistry in the context of precipitation regimes.

To improve understanding of how time-since-fire alters the impacts of pyrogenic material transported into river corridors, we will establish four wildfire chronosequences in the Columbia River Basin (CRB) with wildfires in 6 age classes (1990-present). We will schedule seasonal sampling events to align with different hydrologic conditions (four per year). Additional sampling will occur following at least one large precipitation event per year, per chronosequence. Source (upland soil, charcoal), sediment, porewater, and surface water samples will be collected for analysis of key biogeochemical features (e.g., inorganic nutrients and PyOM indicators) as well as biogeochemical process rates in response to leached source material from each wildfire age. We will also conduct rapid response efforts following new wildfires and precipitation events to evaluate immediate impacts of new wildfires and precipitation events.

Rapid response efforts will allow collection of source material, sediment, porewater, and surface water for biogeochemical analyses that would otherwise be inaccessible.

Additionally, to provide a foundation for how watershed features influence relationships between wildfires, precipitation, and biogeochemistry, we will determine key watershed features at each site, such as stream order and discharge, soil physical properties, surrounding landscape slope, and burn area for initial evaluation of how watershed features influence wildfire impacts on river corridors. We will use machine learning (e.g., random forests and support vector machines) to uncover specific watershed features associated with wildfire age that impact biogeochemical processes.

These activities will generate mechanistic knowledge of how time-since-fire impacts river corridor biogeochemistry in the context of precipitation events and watershed features. They will inform the incorporation of wildfire impacts into predictive models from reaction- to basin-scale.

Novel Insights into Reaction-Scale Biogeochemistry in River Corridors and its Response to Wildfire

Allison Myers-Pigg[1,2*], Vanessa Garayburu-Caruso[1], Swatantar Kumar[1], Bob Danczak[1], Kevin Bladon[3], James Stegen[1], and Emily Graham[1,4]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]Marine Sciences Laboratory, Pacific Northwest National Laboratory, Sequim, WA; [3]Oregon State University, Corvallis, OR; [4]Washington State University, Richland, WA

Contact: (allison.myers-pigg@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to explicate universal indicators of pyrogenic organic matter (PyOM) and to identify the effects of burn severity on relationships between pyrogenic material (e.g., PyOM and inorganic nutrients) and river corridor biogeochemistry. The investigation of wildfires is a critical consideration given increases in wildfire prevalence in the Columbia River Basin (CRB) and is a new aspect of the PNNL SFA—however, we will leverage our previous work in river corridor biogeochemistry, and in particular, the significant role that organic matter chemistry plays in river corridor biogeochemistry. In the new triennial period, we will leverage this expertise, as well as our experience in disturbance ecology, to investigate the impacts of chemical changes associated with varying levels of burn severity. Generally, wildfire- impacted river corridors have elevated concentrations of phosphorus, nitrogen, PyOM, and contaminants. PyOM, in particular, is chemically diverse and has poorly understood biogeochemical implications. Additionally, the effects of combustion temperature on PyOM chemistry and inorganic nutrient concentrations can vary considerably with source material.

To evaluate the impacts of pyrogenic materials across burn severities in the CRB, we will first use laboratory experiments to define typical features of PyOM across burn severities and source materials. Natural substrates from the CRB (e.g., plant materials, upland soils) will be combusted in oxic conditions for two hours across a range of temperatures representative of different burn severities. We will use machine learning to associate known (e.g., polycyclic aromatic hydrocarbons (PAHs), anhydrosugars) and new (e.g., FTICR-MS, GC-MS, NMR-derived) chemical markers of PyOM. Then, we will use laboratory-burned PyOM in controlled experiments to evaluate how inorganic nutrient concentration and PyOM concentration and composition are impacted by different burn severities and how these factors, in turn, influence river corridor biogeochemical rates. Finally, we will conduct sampling across recent fires spanning different burn severities at four locations in the CRB to characterize the natural distribution of PyOM indicators, their impact on biogeochemical processes, and their relationship to watershed features. For site selection, we will leverage 363 wildfires (23,909 km^2) between 2015 and 2017, which span low to high burn severities. At all sites, we will analyze variation in biogeochemical process rates across burn severities and their association with PyOM indicators, inorganic nutrient concentrations, microbial information, and watershed features.

Collectively, these activities will allow us to determine biochemical indicators of PyOM and to identify the impacts of burn severity on river corridor biogeochemistry.

River Corridor Hydrobiogeochemistry Across Basins

James Stegen[1*], Evan Arntzen[1], Scott Brooks[2], Xingyuan Chen[1], Vanessa Garayburu-Caruso[1], Amy Goldman[1], Jesus Gomez-Velez[3], Emily Graham[1], Bob Hall[4], Dan Kaplan[5], Matt Kaufman[1], Hyun Song[6], Ken Williams[7], and Kelly Wrighton[8]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Vanderbilt University, Nashville, TN; [4]University of Montana, Polson, MT; [5]Savannah River National Laboratory, Aiken, SC; [6]University of Nebraska-Lincoln, Lincoln, NE; [7]Lawrence Berkeley National Laboratory, Berkeley, CA; [8]Colorado State University, Fort Collins, CO

Contact: (james.stegen@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA seeks to combine existing global datasets with WHONDRS-based data generation and numerical modeling distributed across the CONUS to discover transferable principles that integrate dissolved organic matter (DOM) chemistry, microbial gene expression, and biogeochemical function in natural and disturbed environments. This campaign leverages community-based approaches to extend our core research objectives across the CONUS. In addition to evaluating transferability of Columbia River Basin knowledge to other basins, the campaign will further establish SBR as a global leader in open watershed science, including a new cross-SBR-SFA initiative to facilitate transferrable knowledge among SBR test beds.

There are five WHONDRS-based research activities in this campaign that all extend PNNL SFA efforts into multiple basins across the CONUS or to the global-scale. The first activity will analyze and model relationships among DOM chemistry, microbial gene expression, and aerobic respiration rates using data generated via previous globally distributed WHONDRS sampling campaigns. The second will use global data from previous and ongoing WHONDRS campaigns to study DOM chemistry to reveal globally consistent and context-dependent (and disturbance- impacted) chemical properties. The third activity will evaluate the degree to which NEXSS predictions of gradients in sediment respiration across stream orders hold across multiple CONUS basins. The fourth activity will pursue a multi-scale analysis (spanning within-reach, within-basin, and among-basin scales) to reveal how variation in DOM chemistry and microbial gene expression change across scales. In addition, these analyses will include a temporal component to characterize among-season changes in levels of variation across scales. The fifth activity will apply a basin-scale river corridor modeling framework--developed in the SFA's 'cumulative impacts' campaign--to multiple basins across CONUS. Applying the basin-scale modeling framework that integrates DOM chemistry, microbial gene expression, and wildfire impacts across CONUS basins will provide key information on how the framework needs to be modified so it can be easily used across basins. This is a key step towards using a basin-scale framework to inform (or potentially integrate with) CONUS-scale (e.g., the national water model) and global-scale (e.g., the land component of E3SM) models.

Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems (WHONDRS)

Amy Goldman[1*], Vanessa Garayburu-Caruso[1], Xingyuan Chen[1], Emily Graham[1], Tim Scheibe[1], Kelly Wrighton[2], and James Stegen[1]

[1]Pacific Northwest National Laboratory, Richland, WA; [2]Colorado State University, Fort Collins, CO

Contact: (amy.goldman@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov/

This element of the PNNL SFA will identify globally-consistent versus context-dependent distributions of dissolved organic matter (DOM) chemistry, including how physical features and disturbances (particularly wildfire) modulate these distributions. For large-scale models to represent DOM chemistry, DOM characterization is needed across environmentally divergent river corridors and factors that drive variation in DOM chemistry need to be understood. Global- scale WHONDRS data indicates that organic molecules (i.e., metabolites) that comprise DOM and that occur in <%5 of rivers (i.e., the transient metabolome) have molecular formulae with relatively consistent elemental ratios. These data also show that the core metabolome (i.e., molecules within DOM that occur in >95% of rivers) has relatively consistent elemental stoichiometry. What is not yet known is whether chemical features (elemental ratios, thermodynamics) of the transient metabolome are organized by environmental features such as stream order or vegetation, and the degree to which disturbances impact chemical properties of the transient and core metabolomes.

We will use data from previous and ongoing WHONDRS sampling campaigns to understand factors leading to coherence and variation in chemistry of both the transient and core metabolomes. This will be done by quantifying distributions of elemental ratios, thermodynamic properties, and inferred biochemical transformations across global samples. Machine learning (e.g., regression trees) will be used to relate differences in transient/core metabolome chemistry to environmental factors such as stream order, disturbance history (e.g., time-since-wildfire, flow variability), and watershed characteristics (e.g., area, net ecosystem productivity, vegetation). As part of this effort, we will continue community-enabled collection of WHONDRS sampling kits to continue to expand the environments across which metabolomes and associated microbial communities and geochemistry are characterized. An area of emphasis will be sampling in coordination with other SBR SFAs immediately following post-fire rainfall events due to the large influence of these events on transporting pyrogenic materials into river corridors. To do so, we will organize 'rapid response' teams ahead of time in areas likely to experience wildfire. The resulting data will be used to evaluate the degree to which wildfire alters river corridor metabolomes and associated features (e.g., does wildfire alter elemental ratios of individual DOM molecules, relative to globally consistent elemental ratios and do microbial communities change simultaneously). This information will fill fundamental knowledge gaps that currently impede our ability to properly represent DOM chemistry and microbial communities in hydrobiogeochemical models.

Understanding Spatial Patterns and Impacts of Hydrologic Exchange and Microbial Community Function from Reaction to Basin Scales

Jesus Gomez-Velez[1*], Kelly Wrighton[2], Xingyuan Chen[3], James Stegen[3], Emily Graham[3], Tim Scheibe[3] and the PNNL SBR SFA Team

[1]Vanderbilt University, Nashville, TN; [2]Colorado State University, Fort Collins, CO; [3]Pacific Northwest National Laboratory, Richland, WA

Contact: (tim.scheibe@pnnl.gov)
Project Lead Principal Investigator (PI): Tim Scheibe
BER Program: SBR
Project: PNNL SBR SFA
Project Website: https://sbrsfa.pnnl.gov

The PNNL SBR SFA is employing principles of ICON/FAIR science and iterative multiscale model-data integration (multiscale ModEx) to build observational networks and numerical models that will enable predictive understanding of river corridor processes from reaction to basin scales. Hydrologic exchange flows (HEFs) and inputs of DOM (amount and molecular properties), nutrients, and contaminants are becoming widely recognized as key factors that influence microbially-mediated reactions in river corridors. However, these factors and responses vary tremendously through space and time across large river basins, making it very difficult to predict their cumulative impacts at watershed to basin scales. We are taking advantage of recent advances in theory, observational capabilities, and numerical modeling to develop interconnected observational networks across multiple large basins in the contiguous U.S. (CONUS) linked to multiscale numerical models in an iterative learning cycle. The NEXSS model has been used to predict HEFs and associated reaction potential across the CONUS, leading to new hypotheses about their distribution across river networks. This information will be combined with basin- scale functional classification of individual catchments using machine learning (ML) to guide the design of field observations and sample collection based on community-based open science approaches developed by the WHONDRS consortium. Resulting metagenomics and metabolomics data will inform reaction-scale models in PFLOTRAN using new theory, KBase workflows, and ML-based surrogate modeling being developed in collaboration with an SBIR project and the IDEAS project. Execution of these models, driven by local estimates of inputs derived from watershed model predictions and tested using laboratory experiments, will generate spatially-distributed estimates of locally-tailored reaction rates, extensible to non-sampled locations based on catchment properties (functional classification). These will, in turn, be assimilated into our river corridor modeling system (MRMT-SWAT-R) to produce updated predictions of basin-scale cumulative effects of river corridor reactions. These updated predictions will be used to refine hypotheses and observational network design, thus completing the iterative cycle of multiscale ModEx. The explicit integration of new reaction-scale understanding into watershed models in this manner offers the potential to quantify cumulative influences of HEFs and molecular properties with enhanced and robust predictive power.

Subsurface Biogeochemical Research

SLAC
SBR Science Focus Area

SLAC Groundwater Quality SFA Program Overview

Kristin Boye,[1*] Christopher Francis,[2] Kate Maher,[2] Scott Fendorf,[2] Kenneth H. Williams,[3] and John R. Bargar[1]

[1]SLAC National Accelerator Laboratory, Menlo Park, CA

[2]Stanford University, Stanford, CA

[3]Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Contact:(kboye@stanford.edu; bargar@slac.stanford.edu) **Project Lead Principle Investigator (PI):** John Bargar **BER Program**: SBR

Project: SLAC Groundwater Quality SFA (John Bargar)
Project Website: https://www-ssrl.slac.stanford.edu/sfa/groundwater-quality-science-focus-area

Project Abstract: Alluvial groundwater is a critical and overdrawn resource in the Western U.S. that supplies water for ecosystem functions and human use. The composition of groundwater is modified by myriad biotic and abiotic sediment-water reactions as it flows through alluvium. Biogeochemical reactivity is concentrated at interfaces between interbedded coarse- and fine- grained sediments, producing sharp redox gradients and biogeochemical (BGC) hot spots and hot moments, *i.e.,* where intensified BGC activity and productivity substantially modify groundwater composition. These subsurface inferfaces may be very large, spanning 10s of square km across a watershed, and thus have major impacts on water quality. Yet in spite of their apparent importance, the mechanisms by which hydrological tiggers such as ET-driven flow or inundation events interact with subsurface interfaces to create BGC hot moments and hot spots, and the resulting impacts on groundwater quality, remain poorly understood and therefore difficult to predict.

The SLAC Groundwater Quality SFA addresses the fundamental question, “How do subsurface interfaces mediate molecular-scale processes and groundwater quality in floodplains and watersheds?” We will systematically investigate molecular to meter scale processes that couple hydrology to BGC and influence groundwater quality using geochemical, microbiological, and hydrological measurements, integrated through reactive transport modeling. We focus on two types of interfaces that are profoundly important to water quality and floodplain BGC function, but which have received little research attention at the molecular-to-system level: (1) Interfaces between coarse (gravel/cobble) basal alluvium and overlying fine-grained organic-rich sediments, which are ubiquitous and extends over large areas in mountain and intermountain West riparian corridors, as exemplified by two uranium- and metals-contaminated field sites at Slate River, CO and Riverton, WY. These interfaces appear to be ‘hot spots’ for the generation of colloids carrying Fe, S, Mn, organic carbon, and trace metals, indicating their importance as sources for colloidal transport and associated implications for water quality. (2) Fine-grained, reducing sediment lenses and layers embedded within coarse-grained aquifer material with low groundwater oxygen concentrations (but not anoxic), which promote the establishment of ‘reducing halos’ in the aquifer material and profoundly alters groundwater composition. We are developing quantitative process representations that will contribute directly to the IDEAS-Watershed ESS software ecosystem. This work will provide new and deeper mechanistic process knowledge of hydrological-BGC coupling within floodplains and watersheds, their impact on water quality, and their response to changing weather patterns and other perturbations.

SLAC Groundwater Quality SFA: Linking Riparian Microbial Communities and Biogeochemical Cycling to Vertical Groundwater Flow Across Oxic-Anoxic Interfaces at Slate River, CO

Bradley B. Tolar,[1,2*] Christian Dewey,[1] Tristan Babey,[1,2] John R. Bargar,[2] Samuel W. Pierce,[2] Scarlet-Marie Kilpatrick,[1] Andrew H. Manning,[3] Kenneth H. Williams,[4] Kate Maher,[2] Scott Fendorf,[1] and Christopher A. Francis[1]

[1]Stanford University, Stanford, CA

[1]SLAC National Accelerator Laboratory, Menlo Park, CA

[3]Geology, Geophysics, and Geochemistry Science Center, US Geological Survey, Denver, CO

[4]Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: (btolar1@slac.stanford.edu)

Project Lead Principle Investigator (PI): John Bargar

BER Program: SBR

Project: SLAC Groundwater Quality SFA (John Bargar)
Project Website: https://www-ssrl.slac.stanford.edu/sfa/groundwater-quality-science-focus-area

Project Abstract: Riparian floodplains along Slate River in Gunnison County, CO are contaminated by heavy metals leached from mine operations. Fine-grained riparian sediments are anoxic and veneer underlying oxic basal gravel aquifer, creating a sharp *inverted* oxic-anoxic transition. Field measurements and hydrological modeling indicate that summer ET drives upward groundwater flow, carrying oxic groundwater from the basal gravel bed into overlying fine-grained anoxic sediments and creating biogeochemical hot zones that condition ground- and river water quality. We have observed intense redox cycling in the fine sediments, generation of metal-organic colloids, and mobilization of Fe, Mn, organic C, Zn, and Pb. Riparian flood plains are aerially extensive (10s of km^2 in the upper Slate River watershed) and their gravel beds are well connected to adjacent rivers. Moreover, gravel beds are the dominant river-bed form throughout the intermountain West. It therefore likely that these coupled hydrological-biogeochemical processes influence watershed scale trace metal and nutrient behavior across this large region.

We posit that metabolic and community responses of riparian microorganisms to variations in the composition of vertically flowing groundwater control mechanistic linkages between hydrology and biogeochemistry. To lay the foundation for studies of groundwater triggers and microbial responses, we collected vertical profiles of sediments and pore-water in riparian sediments along Slate River for geochemical and microbial analyses. Using 16S rRNA amplicons obtained from sediment DNA extracts, we observed aerobic microorganisms (including nitrifiers) at depths ≤90 cm, while anaerobic microorganisms (including methane- and sulfur-cycling groups) reside only in the deepest depths (130-150 cm). A well-defined aerobic (above)-anaerobic (below) transition was observed within the saturated zone of the fine sediments at ~110 cm depth. This zone appears to harbor members of both aerobic and anaerobic communities, suggesting that this depth also likely experiences fluctuating oxygen conditions. The microbial groups identified can mediate biogeochemical reactions that mobilize metal contaminants and play a role in extensive Fe-bearing colloid formation observed in the anoxic zone. These findings offer a new view of alluvium- groundwater dynamics and microbial community responses. Further investigation of these dynamics alongside microbial community data will enhance our understanding of the drivers of biogeochemical cycling at oxic/anoxic transition zones.

SLAC Groundwater Quality SFA: Host Recalcitrance Protects Against Pb Mobilization in Floodplain Sediments During Seasonal Redox Cycles

Christian Dewey,[1*] Samuel W. Pierce,[2] Scott Fendorf,[1] and John R. Bargar[2]

[1]Stanford University, Stanford, CA

[1]SLAC National Accelerator Laboratory, Menlo Park, CA

Contact: (cwdewey@stanford.edu)

Project Lead Principle Investigator (PI): John Bargar

BER Program: SBR

Project: **Project**: SLAC Groundwater Quality SFA (John Bargar)

Project Website: https://www-ssrl.slac.stanford.edu/sfa/groundwater-quality-science-focus-area

Project Abstract: Understanding the controls on sequestration and mobilization of heavy metals is essential for assessing the risk they pose to water quality. We examined the impacts of seasonal redox cycles on Pb speciation and potential mobility in sediments in the Slate River floodplain (near Crested Butte, CO), which is affected by several hard-rock mines. Through a combination of field measurements, X-ray absorption spectroscopic techniques, and sequential extractions, we find that, above the baseflow water table elevation, where sediments are unsaturated and oxidized, Pb within the solid phase occurs predominantly as surface complexes on goethite (Pb-Gt) and particulate organic matter (Pb-POM). Below the baseflow water table, where sediments are reduced, Pb occurs predominantly as galena (PbS) and Pb-POM and, to a lesser extent, Pb-Gt. In porewater from both unsaturated and saturated sediments, Pb concentrations do not exceed 5 ppb over a 5-month period, indicating that dissolved Pb is not mobilized in either zone (unless during undetected transient moments). As river discharge increases seasonally, sediments become saturated above the baseflow water table elevation, transitioning oxidized sediments into reducing conditions. We observe iron and sulfate reducing conditions develop as oxidized sediments become reduced, revealed by an increase in Fe(II)(aq) concentrations and the formation of sulfidic phases. With the return to baseflow conditions, sediments are re-oxidized. Throughout these redox cycles, Pb speciation changes minimally, and pore water Pb concentrations remain below 5 ppb, indicating that, in seasonally reduced sediments, partitioning of Pb to goethite and POM limits dissolved Pb concentrations and the formation of PbS. Further, the abundance of PbS in permanently saturated (and reduced) sediments indicates that prolonged (i.e., on the order of years, decades, or longer) reducing conditions are required for authigenic PbS formation and/or preservation of geogenic PbS. Together these findings reveal that partitioning to solid phases limits dissolved Pb mobilization, while long-term redox regimes, established by baseflow water table elevation, control Pb speciation. Finally, these findings illustrate that colloid-forming processes and sediment transport are the principal threats to water quality.

SLAC Groundwater Quality SFA: Simulations of Anoxic Lenses as Exporters of Reactivity in Alluvial Sediments

Tristan Babey,[1*] Kristin Boye,[1] Zach Perzan,[1] John R. Bargar,[2] and Kate Maher[1]

[1]Department of Earth System Science, Stanford University, Stanford, CA;

[2]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA;

Contact: (tbabey@stanford.edu)

Project Lead Principle Investigator (PI): John Bargar

BER Program: SBR

Project: DOE SFA program (J. Bargar), DOE SBR IDEAS-Watersheds Project

Project Website: https://www-ssrl.slac.stanford.edu/sfa/groundwater-quality-science-focus-area

Project Abstract: Understanding the development of mixing zones between contrasting hydrogeological facies is critical to predict the transfer and mobilization/retention of contaminants. This is the case for gravel bed alluvial aquifers in the intermountain West, which often exhibit both complex sedimentary structures and contamination derived from human activity or geogenic sources. The juxtaposition of fine-grained, organic matter enriched sediments with more permeable aquifer material is an important property in these systems and has been observed to profoundly alter the mobility of redox-sensitive elements such as O_2, Fe and S. In spite of the importance of those interfaces to water quality, quantitative process representations of the various physical and biogeochemical processes involved do not exist, and the characterization of how their coupling modulates groundwater geochemistry remains as an ongoing challenge.

Here we calibrate a reactive transport model on a series of column experiments using sediments from a field site at Riverton, WY, where low-permeability, organic-rich reducing lenses (Naturally Reduced Zones, NRZs) are embedded in coarser-grained aquifer material. Simulations are carried out in water-saturated conditions using the numerical reactive transport code CrunchFlow. They explicitly account for C, O_2, Fe and S cycling at the interface between NRZs and the aquifer. Simulation results highlight the role of NRZs not only as sources or sinks for redox-sensitive species, but also as exporters of reactivity. By releasing large amounts of organic carbon into the surrounding aquifer, NRZs drive the development of secondary reduction zones, or "halos", in their vicinity, characterized by high microbial activity (e.g. sulfate reduction) and the accumulation of reduced reaction products (e.g. iron sulfide mineral). Because those secondary reduction zones are hydraulically connected to the aquifer, they are susceptible to changes in hydrologic conditions, for instance oxygen pulses associated with seasonal snowmelt. Our results also emphasize the limitations of relying solely on aqueous species measurements to inform reactivity in such systems: high precipitation rates of iron sulfide minerals (mackinawite) combined with sizeable transport of organic carbon presumably in colloidal form lead to a limited signature of reactivity in the dissolved phase.

SLAC Groundwater Quality SFA: Preferential Mobilization of Nutrients Driven by Distinct Forms of Inundation on a Semi-Arid Floodplain

Zach Perzan,[1*] Kristin Boye,[2] Callum Bobb,[1] Kate Maher,[1] and John Bargar[2]

[1]Stanford University, Stanford, CA

[2]SLAC National Accelerator Laboratory, Menlo Park, CA

Contact: (zperzan@stanford.edu)

Project Lead Principle Investigator (PI): John Bargar

BER Program: SBR

Project: SLAC Groundwater Quality SFA (John Bargar)

Project Website: https://www-ssrl.slac.stanford.edu/sfa/groundwater-quality-science-focus-area

Project Abstract: Floodplains are a central link in the transfer of nutrients between landscapes; they can retain, transform, or release nutrients as solutes move between the terrestrial and riverine ecosystems. In arid and semi-arid environments, seasonal floods are short-duration events that have an outsized impact on the annual flux of nutrients between these two systems. Though flood frequency and duration are often considered the most important factors in determining floodplain nutrient fluxes, other elements of inundation – especially the source of inundated water – play a role as well.

To examine the relative impact of each of these factors, we monitored porewater solute concentrations during multiple types of inundation events on a semi-arid floodplain in Riverton, WY. Observations from the site over the 2017, 2018, and 2019 field seasons show that the Riverton floodplain experiences two main drivers of inundation: water table rise and surface ponding. In an inundation event driven by water table rise, rising river stage increases hydraulic head such that the water table within the floodplain rises to the surface. By contrast, in an inundation event driven by surface ponding, water pools up on the surface during intense precipitation, then percolates downward through the vadose zone to the water table.

Surface ponding events result in limited downward flushing of vadose zone nutrients, as water percolating through the unsaturated zone flows primarily along preferential flow paths. Water table rise events, on the other hand, result in complete saturation of the soil profile, but may or may not flush nutrients from the vadose zone, depending on the composition of the inundated water. Our results suggest that monitoring flood frequency and duration is not adequate for understanding subsurface response to inundation events; other factors – including antecedent soil moisture, the driver of inundation, and the composition of inundated water – need to be taken into account for a complete understanding of floodplain nutrient fluxes.

SLAC Groundwater Quality SFA: Describing and Quantifying Anaerobic Microsites: Impact on BGC Nutrient Cycling in Soils

Vincent Noël,[1*] Sam Webb,[1] Kristin Boye,[1] Kate Maher,[2] Chris Francis,[2] Scott Fendorf,[2] and John R. Bargar[1]

[1]SLAC National Accelerator Laboratory, Menlo Park, CA;

[2]Stanford University, Stanford, CA

Contact: (noel@slac.stanford.edu)

Project Lead Principle Investigator (PI): John Bargar

BER Program: SBR

Project: SLAC Groundwater Quality SFA (John Bargar)

Project Website: https://www-ssrl.slac.stanford.edu/sfa/groundwater-quality-science-focus-area

Project Abstract: Anaerobic soil heterogeneities, referred to as 'anaerobic microsites', form in aerated soils where textural contrasts create boundaries defining small (µm to mm diam) domains in which oxygen consumption exceeds inward O_2 flux. A widely posited function of these features is to maintain anaerobic disequilibrium within nominally oxic soil horizons. Thus, anaerobic soil microsites have been widely invoked, but rarely observed and characterized, to explain the presence of reduced products that otherwise should be absent from the soil system. BGC functions ascribed to microsites include organic carbon storage, denitrification and ammonification, manganese/iron/sulfur reduction, methanogenesis, and metal contaminant sequestration/release. Neglecting to account for anaerobic microsites in soils creates major uncertainties in model simulations of greenhouse gas emissions, stable isotope fractionation, and nutrient and contaminant transport. In spite of their importance, we know little about the physical, geochemical, and microbiological characteristics of anaerobic microsites, particularly their distributions within soil horizons and their impacts on the compositions of soil water/gas and the atmosphere.

This lack of knowledge is due mainly to instrumental limitations that constrain our ability to detect and characterize these small soil features. In a new project, we will use synchrotron-based X-ray imaging to address the question of, "When, where, how, and to what extent do anaerobic microsites contribute locally and globally to ecosystem functions (and to which ones?)". When coupled with X-ray spectroscopy, this method offers unique abilities to detect redox contrasts and the distribution of specific elements (including S, Fe, Mn, As, U, Cr, Mo) *and their oxidation states and chemical forms* within soil cores at spatial resolution extending down to micron-scale. We will adapt, optimize, and integrate existing synchrotron X-ray methods into a workflow for detecting and characterizing anaerobic soil microsites. We will work closely with DOE-ESS collaborators to evaluate the importance of detected anaerobic microsites on varying biogeochemical function in focus for ESS funded researchers. If successful, the project will inform process knowledge of, and ability to model, the broad and critical BGC roles played by anaerobic microsites across terrestrial ecosystems.

Scientific User Facilities and Community Resources

Title: **The Third ARM Mobile Facility: Coupled Observational-Modeling Studies of Land-Aerosol-Cloud Interactions in the Southeastern United States**

Chongai Kuang[1*], Shawn Serbin[1], Scott Giangrande[1], Gregory Elsaesser[2,3], Pierre Gentine[3], Thijs Heus[4], Michael Jensen[1], Pavlos Kollias[1,5], Allison McComiskey[1], Hugh Morrison[6], Mariko Oue[5], John Peters[7], Markus Petters[8], Arthur Sedlacek[1], James Smith[9], Allison Steiner[10], David Turner[11], Andrew Vogelmann[1]

[1]Environmental & Climate Sciences Department, Brookhaven National Laboratory, Upton, New York

[2]NASA Goddard Institute for Space Studies, New York, NY

[3]Columbia University, New York, NY

[4]Cleveland State University, Cleveland, OH

[5]Stony Brook University in New York, Stony Brook, NY

[6]NCAR, Boulder, CO

[7]Naval Postgraduate School, Monterey, CA

[8]North Carolina State University, Raleigh, NC

[9]University of California, Irvine, Irvine, CA

[10]University of Michigan, Ann Arbor, MI

[11]NOAA, Boulder, CO

Contact: (ckuang@bnl.gov)

Project Lead Principal Investigator (PI): Chongai Kuang

BER Program: ARM, ASR

Project: User Facility, DOE Lab-led project

Project Website: https://arm.gov/news/facility/post/59923

Project Abstract:

The U.S. Department of Energy's Atmospheric Radiation Measurement (ARM) user facility will be relocating the third ARM Mobility Facility (AMF3) to the Southeastern United States (SEUS) for a five-year deployment starting in the fall of 2022. The AMF3 SEUS site science team is working with ARM and the larger scientific community to guide the siting of the new deployment in order to address critical science focal areas spanning five cross-cutting topics: convective cloud initiation, deep convective cloud processes, aerosol controls on cloud condensation nuclei, aerosol direct impacts on radiation, and land-atmosphere two-way interactions (LAI). Of particular interest to the ESS community, the LAI focus will target key cross-cutting topics including the strong local coupling of the land-surface with atmospheric processes, surface-atmosphere feedbacks, influence of regional heterogeneity on land-surface modeling, and the influence of surface dynamics on regional aerosol formation. This deployment will enable a wide range of observational, analysis, and modeling studies to characterize the relationships between local and regional weather patterns and surface processes across a patchwork of natural, managed, and anthropogenic landscapes in the SEUS region.

The Brookhaven National Laboratory-led team will develop a science plan and perform initial research activities for the AMF3 deployment in the SEUS. This team will:

- inform AMF3 deployment and science strategies by conducting modeling studies, observation system simulation experiments and analysis of existing measurements,
- identify potential deployment locations,
- provide scientific input on site layout and instrumentation needs,
- develop new analysis algorithms, data sets, and software tools,
- identify and develop collaborations with partners in the SEUS,
- lead outreach within the broader research community for location, site design, and use promotion, and
- coordinate and conduct initial process-based research activities.

Title: EMSL: A DOE Office of Science User Facility for Environmental System Science Research

Nancy Hess[1]*, Chris Anderton[1], Pubudu Handakumbura[1], Jim Moran[1], and Tamas Varga[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 that leads to identifying key microbial, biogeochemical, and hydrologic processes that control species reactivity and mobility across multiple spatial and temporal scales. Probing these dynamic processes at molecular scale provides mechanistic information to accurately represent these processes in computational reactive flow and transport models or community land models —an important goal of many Environmental System Science researchers who address the nation's environmental and energy challenges. Linking experimental and theoretical approaches from molecular to field scales requires the convergence of diverse experimental and computational techniques, plus collaboration with experts from multiple disciplines.

At EMSL, we provide expertise for scientific studies and discovery with our integrated experimental, computational, and modeling and simulation resources. A few hot areas of community research include understanding the chemical fate and mobility of contaminants in the biogeochemical environment; the role of microbial communities driving nutrient cycling in the rhizosphere; the speciation of metal ions and complexes on surfaces, in solution, or incorporated into mineral phases; unraveling the molecular messaging between microbes, plants, soil, and geochemistry; and investigating plants' molecular phenotypic responses to environmentally controlled stressors, including temperature, water availability, light cycles, and CO_2 levels.

We are expanding capabilities to couple computational resources with data generation for knowledge generation. We are also pairing 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. Additionally, we are performing genomic sequence analysis and data mining to improve the depth of coverage from proteomics studies. Our extensive expertise 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.

Access to resources at EMSL for environmental and biological sciences is free of charge to the research community and granted through a peer-review proposal process (www.emsl.pnl.gov/emslweb/proposal-opportunities).

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

Susannah Tringe,[1]* David Gilbert[1], Nigel Mouncey[1]

[1]DOE Joint Genome Institute, Lawrence Berkeley National Laboratory, Berkeley, CA

Contact: sgtringe@lbl.gov

Project Lead Principal Investigator (PI): Nigel Mouncey

BER Program: User Facility

Project: User Facility

Project Website: http://www.jgi.doe.gov

Project Abstract:

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 joint calls with other DOE user facilities through the Facilities Integrating Collaborations for User Science (FICUS) program. These include collaborative programs with the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (PNNL) enabling molecular characterization and imaging in concert with genomics and with the National Energy Research Scientific Computing Center (NERSC) providing computational capacity and expertise. 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.

Title: The Surface Atmosphere Integrated field Laboratory (SAIL) ARM Mobile Facility Campaign

Daniel Feldman[1,*], Allison Aiken[2], William Boos[3], Rosemary Carroll[4], Venkatachalam Chandrasekhar[5], William Collins[1,3], Scott Collis[6], Jeffrey Deems[7], Paul DeMott[5], Jiwen Fan[8], Alejandro Flores[9], Dave Gochis[10], Jerry Harrington[11], Matthew Kumjian[11], L. Ruby Leung[8], Travis O'Brien[12], Mark Raleigh[13], Alan Rhoades[1], McKenzie Skiles[14], James Smith[15], Ryan Sullivan[6], Paul Ullrich[1,16], Adam Varble[8], Kenneth Williams[1]

* Presenting Author

[1] Lawrence Berkeley National Laboratory, Berkeley, CA

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

[3] University of California-Berkeley, Berkeley, CA

[4] Desert Research Institute, Reno, NV

[5] Colorado State University, Fort Collins, CO

[6] Argonne National Laboratory, Lemont, IL

[7] National Snow Ice Data Center, Boulder, CO

[8] Pacific Northwest National Laboratory,

[9] Boise State University, Boise, ID

[10] National Center for Atmospheric Research, Boulder, CO

[11] Pennsylvania State University, State College, PA

[12] Indiana University, Bloomington, IN

[13] Oregon State University, Corvallis, OR

[14] University of Utah, Salt Lake City, UT

[15] University of California-Irvine, Irvine, CA

[16] University of California-Davis, Davis, CA

Contact: (drfeldman@lbl.gov)

Project Lead Principal Investigator (PI): Daniel Feldman BER Program:

ARM

Project: User Facility

Project Website: http://www.arm.gov/campaigns/amf2022sail

Project Abstract:

The Surface Atmosphere Integrated field Laboratory (SAIL) campaign will involve the deployment of the U.S. Department of Energy's Atmospheric Radiation Measurement program's second mobile facility (AMF2) in the vicinity of Crested Butte, Colorado from September 2021 to June of 2023. This atmospheric observatory will measure surface fluxes of momentum, sensible and latent heat, the spatial distribution of precipitation and winds, temperature, humidity, aerosol and cloud properties, and radiation; and it will develop this detailed dataset by while being collocated with existing surface and subsurface observations and modeling from the SBR-funded Watershed Function SFA.

The dozens of unique atmospheric datastreams from SAIL, along with observations of streamflow, vegetation distribution, snowpack, and a suite of hydrometeorological conditions from stations across the 300 km^2 East River Watershed developed by the Watershed Function SFA, will enable SAIL to address the following science objectives:

1. Characterize the spatial distribution of orographic and convective precipitation processes on diurnal to seasonal time-scales and how those processes interact with large-scale circulation.
2. Quantify cold-season land-atmosphere interactions that alter snowpack mass balance through wind redistribution and sublimation and the spatial scaling of those processes.
3. Establish aerosol regimes, the processes controlling the life cycle of aerosols in those regimes, and quantify the impacts of aerosols in those regimes on the atmospheric and surface radiative budget.
4. Quantify the sensitivity of cloud phase and precipitation to cloud condensation nuclei (CCN) and ice-nucleating particle (INP) concentrations
5. Quantify the seasonally-varying surface energy balance, the land-surface and atmospheric factors controlling it, and the spatial variability in those factors.

In addressing these objectives, SAIL will advance the characterization and modeling of the dominant atmospheric processes that impact the mass and energy balance of high-altitude complex terrain watersheds of the Upper Colorado River basin. These data can also benefit surface and sub-surface process-model development by systematically characterizing precipitation inputs, sublimation and evapotranspiration losses, and the components of the surface energy balance.

Small Business Innovative Research (SBIR) Awards

Monitoring Saturated and Unsaturated Environments Using Microbial Potentiometric Sensors (MPS)

Scott Burge[1], Russell Burge[1], Kiril Hristovski[2] [1]Burge

Environmental Inc. Tempe, AZ [2]Arizona State

University, Mesa, AZ

(Burge@burgeenv.com)

Project Lead Principal Investigator (PI): Scott Burge BER

Program: SBIR/STTR

Project: SBIR (Rhizosphere Monitoring) Project

Abstract:

The further development of the MPS system has enabled the direct interrogation of subsurface environments using biofilms that populating the surface of the sensors. The sensors require no maintenance or calibration and are ideal for long-term monitoring programs. The sensors are deployed in large arrays (200-300 sensors) to provide 3D-visualizations of the electrical potential within the subsurface environment. The sensor arrays connect to a solar-powered signal acquisition/communication (cellular) circuitry. The data are transmitted and stored in cloud-base storage system and downloaded by the user into open-source dashboards and visualization programs. We will present MPS data from several subsurface environments.

Title: **Integrated ChemFET Sensors for Real time Monitoring of Redox Sensitive Metals in Natural Water**

Yuhong Kang[1*], Liz Gladwin[1], Hang Ruan[1], Robert Moore[2], Emily Plunkett[2], Christina Orsino[2]

[1]NanoSonic, Inc. Pembroke, VA
[2]Virginia Tech, Blacksburg, VA

Contact: (ekang@nanosonic.com)

Project Lead Principal Investigator (PI): Dr. Yuhong Kang

BER Program: SBIR

Project: SBIR

Project Website: https://nanosonic.com/

Project Abstract:

Redox sensitive metals - chromium, iron, manganese, and others have attracted a great deal of attention around the world for their impact on human health and the environment. It is beneficial to study the temporal dynamics of metal ion concentrations and coupled biogeochemical reactions. To allow efficient monitoring of redox sensitive metal levels in water, a fast response, field deployable, sensitive and selective measuring instrument is required. Traditionally, there are several methods for heavy metal detection, including spectroscopic techniques such as atomic absorption spectroscopy, Auger-electron spectroscopy, and inductively coupled plasma-mass spectrometry. However, these methods are expensive to use with costly and bulky instruments, and are not suitable for field monitoring applications. The fundamental physical principles of ordered dielectric or metallic thin films formed by the electrostatic self-assembly (ESA) process have been investigated in our team's prior publications. Most importantly, research has demonstrated the ability of ESA to incorporate a wide range of materials including polymers, metal and oxide nanoclusters, cage-structured molecules, semiconductor nanocrystals, and other materials, into multilayered thin films. Applications of these chemically selective thin films in chemical field effect transistors (ChemFET) sensors and integrated systems are suggested.

Experimental data demonstrates miniaturized ChemFET sensors with chemically modified electrodes for the detection of redox sensitive metal ions such as Fe(II), Fe(III), Cr(III), Cr(VI), and others in surface and subsurface water. We have combined our electrostatic self-assembly thin film deposition process and stripping voltammetry enhanced ChemFET technology to produce an integrated chemical sensor network with tuned sensitivity and selectivity for *in situ* environmental monitoring. High selectivity is achieved by designing specific self-assembled binding interfaces for metal ions of interest. The team investigated the issues encountered in groundwater monitoring, which mainly include the difficulty in forming strong and reversible bindings between sensing materials and target metal ions, the interfering ion complexation from natural organic ligands and other chemicals, and the gradual accumulation of microorganisms/other materials on wet sensor surfaces. It leads to improved reversibility and reusability of the sensor systems. The wired/wireless sensor system would be capable of sensing multiple redox sensitive metal ions, improve upon conventional sampling methods, and benefit future environmental analysis programs.

Biogeochemical Characterization of Redox Species in Real time

An *in-situ* instrument that simultaneously collects all relevant redox information from any environmental system

Donald Nuzzio[1*]

[1]Analytical Instrument Systems, Inc., Flemington, N.J. Contact:

dnuzz@mac.com

BER Program: SBR Project:
SBIR

Website: www.aishome.com

Data will be presented for the first time that illustrates the power of this new *in-situ* instrumentation. The ability to collect simultaneous data on the most pertinent biogeochemical species in real time is critical in understanding complex environmental systems. Data collected using the DLK MP-1 instrument at the East River Watershed Colorado location during the last snow melt in 2019 will be presented.

Deployment of this system enabled data collection of data for slightly over a month, with 321,000 data sets collected approximately every 10 seconds. The instrument collected data without interruption, and the electrode sensors have proven to be robust over this time period. The data collected show clear diurnal cycling of the major biogeochemicals and can be also correlated with evapotranspiration in forested areas. The system is also very versatile and can be used in any seawater or freshwater system. This is a true advancement in technology and will change how we collect *in-situ* data in the future.

A cloud based cyberinfrastructure for automated model/data integration

Roelof Versteeg[1*], Haruko Wainwright[2], Nicola Falco[2], Doug Johnson[1], Erek Alper[1], Satish Karra[3], Ye Zhang[4], Peter Lichtner[5], Reza Soltanian[6], Kelly Wrighton[7], Chris Henry[8], Haiyan Zhou[1], Rebecca Rubinstein[1]

[1] Subsurface Insights, Hanover, NH

[2] Lawrence Berkeley National Laboratory, Berkeley, CA

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

[4] University of Wyoming, Laramie, WY

[5] OFM Research, Santa Fe, NM

[6] University of Cincinnati, Cincinnati, OH

[7] Colorado State University, Fort Collins, CO

[8] Argonne National Laboratory, Lemont, IL

Contact: roelof.versteeg@subsurfaceinsights.com

BER Program: SBR

Project: SBIR

Project Website: www.subsurfaceinsights.com

Project Abstract:

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

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

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

PAF has been developed and demonstrated using data from both DOE funded projects and data from other research institutions and the private sector. PAF currently can ingest geochemical, geophysical, hydrological and remote sensed data and uses the PFLOTRAN reactive transport model for modeling and analysis. Both data

and capabilities within PAF can be accessed through browser and mobile interfaces and software APIs, allowing for easy integration with third party computational capabilities. An example of this is our ability to automatically parameterize and run PFLOTRAN models both through a browser, a mobile phone and through an API. Such models can be parameterized and validated through remote sensing and local data. We will discuss and demonstrate how our infrastructure can be used for automated model generation and model/data integration and optimization.