GENOMES TO WATERSHEDS

E-Newsletter for the LBNL Sustainable Systems Scientific Focus Area (SFA)

Issue 2 / Fall 2014

Team and guests of the October 2014 SFA Retreat, Bodega Bay CA

From the Director:

Although only launched in October of 2013, the Berkeley Lab Genome-to-Watershed SFA 2.0 project has made substantial progress along several critical and linked research fronts. Recent examples includes

- Significant advances in quantifying subsurface metabolic potential. Using new bioinformatics approaches, over 1,000 mostly novel subsurface genomes have been sequenced, many involved in N, S, H, C cycling.
- Metatranscriptomics have revealed the inordinate role of chemolithoautotrophy on nitrogen cycling.
- Documented importance of both hot spots and hot moments important to the Rifle CO floodplain biogeochemistry.
- First study to document requirement of genome-informed reaction networks for accurate simulation of the subsurface terrestrial environment.

Information about these and other advances can be found through our publications and presentations. At the **Fall AGU meeting in San Francisco**, project members are leading several sessions and are involved in over 20 genome-to-watershed project presentations. A description of the project's AGU contributions is provided here.

We held a first year retreat at Bodega Bay in October of 2014. The retreat was organized to take stock of our progress and refine plans toward quantifying and predicting terrestrial environment biogeochemisty: from bedrock to canopy and from genome to watershed to river basin scales. All team members attended, as well as several guests, including Nate McDowell, David Moulton, Lara Keuppers, Charlie Koven, Joel Rowland, and John Bargar. The retreat included discussions, presentations and breakout sessions, the latter led by SFA 2.0 early career staff on topics of Upscaling Constructs (Bhavna Arora), vegetation influence on hydrological partitioning (Baptiste Dafflon) and the subsurface carbon budget (Nick Bouskill).

We look forward to seeing many of you at AGU - **Please stop by to visit SFA 2.0 scientists at AGU booth #2309!**

Susan S. Hubbard

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Community Involvement:

Complex Soils Systems Conference: SFA members Eoin Brodie and Boris Faybishenko together with others from LBL organized the September 2014 Complex Soils Systems Conference.

More than 170 scientists from 13 countries attended this event, representing ecology, hydrology, geophysics, agriculture, soil chemistry, soil physics, soil microbiology, mathematics, modeling of soil-climate interactions and other fields.

One of the conference's main goals was to provide a motivating framework toward improved understanding of complex soil systems. The conference offered an important channel for

information exchange between researchers, and provided a turning point for soil science!
Learn more by visiting: Soils Conference

2014 Geological Society of America Annual Meeting in Vancouver, BC.

Phil Long presented a talk on "Predictive understanding of subsurface biogeochemical functioning: using genomes to inform watershed-scale models." as part of the session on how microbial ecology and evolution intersect with biogeochemical cycling, climate change, biogeography, medical geology, and bioremediation. Phil also presented a talk entitled "Depth- and time-resolved temperature of the vadose zone and a shallow alluvial aquifer beneath a Colorado River floodplain" in a session on Dynamics of Groundwater Temperature: From Recharge to Discharge Zones. Phil presented the paper for Boris Faybishenko who was unable to attend the meeting.

SFA member Tetsu Tokunaga was highlighted in a recent **DOE-LM Quarterly Program Update**, describing the unique instrumentation that he has installed at the Rifle CO site to measure moisture dynamics that are critical for understanding contaminant migration. Go here for full report and read further for research updates.

SFA team members gave 18 presentations at the June 2014 **Goldschmidt** meeting in Sacramento, CA, including the following keynote presentations:

- Jill Banfield: Prediction of the Biogeochemical Roles of Uncultivated Bacteria and Archaea in the Subsurface
- Ken Williams: A Floodplain Perspective on Elemental Cycling and Uranium Plume Persistence
- Carl Steefel: The GEWaSC Framework: Multiscale Modeling of Coupled Biogeochemical, Microbiological, and Hydrological Processes"
- Cristina Cismasu: Iron and Carbon Dynamics during the Reductive Transformation of Organic Matter-Rich Fe(III)

RIFLE City Council Meeting June 16, 2014

Phil Long and Ken Williams updated the City of Rifle City Council on the status of research at the Rifle site at a workshop held prior to the formal city council meeting. City council members showed great interest in research at the Rifle site. A lively discussion ensued on a wide range of topics including significance of SFA 2.0 research to the energy extractive industry that is a key part of the local economy. The meeting was also attended by Dick Dayvault of SM Stoller, Inc. representing DOE–LM, Grand Junction.

Research Updates:

JGI awards a third major increment of sequencing to the SFA project:

2,000,000,000,000 (2 Tb) of new sequence data for genomic analysis of subsurface microorganisms.

Based in part on the strength of prior accomplishments that made use of previously awarded sequencing, the Joint Genome Institute recently approved our application for 1 Tb of metagenomic and 1 Tb metatranscriptomic data from subsurface sediment and groundwater samples. A subset of samples has already been collected from a variety of depths through a naturally bioreduced zone in conjunction with drilling activities targeting geophysically-identifed 'hot spots' or so-called biogeofacies (see Image and highlight from Ken Williams). The new sequencing will expand research into the vadose zone and includes a time series of planktonic samples. This effort will increase the amount of sequence information for the Rifle site to around 4 Tb and will provide unprecedented, genome-resolved insight into community structure, the metabolic potential of specific organisms and their contributions to carbon cycling, the geochemical controls on organism distribution and the responses of the system to perturbations.

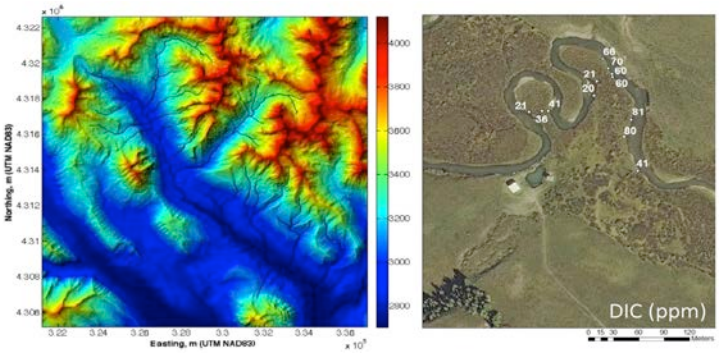
Photograph of sediment collected in August, 2014 for sequencing.

Contributors: **Jill Banfield,** Susan Hubbard, Ken Williams, Harry Beller, Eoin Brodie, Laura Hug, Cindy Castelle, Karthik Anantharaman and others

Floodplain to Watershed: Reconnaissance investigations at the East River Catchment of the Upper Colorado River Basin:

Site scoping activities and preliminary data collection within the East River Catchment suggest its appropriateness as a second field study site for LBNL's SFA 2.0 research program.

Data collection and transport modeling activities were initiated for the East River Catchment (Colorado, USA) to assess its suitability as a second field study site for LBNL's SFA 2.0 research program.



Digital elevation model of the East River Catchment and hyporheic sampling results from floodplain deposits within a subcomponent of the modeling domain.

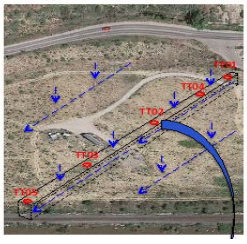
The site of the Rocky Mountain Biological Laboratory, the upper East River Catchment is a 250km^2 headwaters system of the Gunnison River, one the primary tributaries of the Colorado River within the Upper Basin States (CO, WY, NM, UT). Scoping activities initiated in April 2014 include: (a) installation of 12 stilling wells/gaging stations; (b) weekly geochemical sampling at each of the 12 locations; (c) autosamplers collecting daily streamwater samples at 2 locations; (d) hyporheic sampling within floodplain deposits associated with the low gradient, meandering reach; (e) installation of 8 piezometers for groundwater sampling; (f) geophysical data collection at multiple locations within the catchment; (g) data mining and compilation of remote sensing data; (h) installation of sediment traps to quantify deposition rates; (i) analysis of soil/sediment carbon stocks; and (j) initiation of flow and transport modeling activities for the 250km^2 domain. Analytical results and success inmodel initiation suggest the catchment's appropriateness as a second field study site, with an expansion of research activities there planned during FY15.

Contributors: **Ken Williams** and others

Vertically and temporally resolved water flux directions, pore water chemical composition, and CO_2 fluxes in the Rifle floodplain vadose zone and capillary fringe:

Measurements from tensiometers, pore water samplers, and vadose zone gas samplers are yielding new insights into water, carbon and nitrogen cycling in the Rifle subsurface.

Understanding the cycling of water and other chemical components in the environment requires quantification of their fluxes between the atmosphere, soil, vadose zone, and groundwater. We are obtaining such information at the Rifle Site, a semi-arid floodplain along the Colorado River.



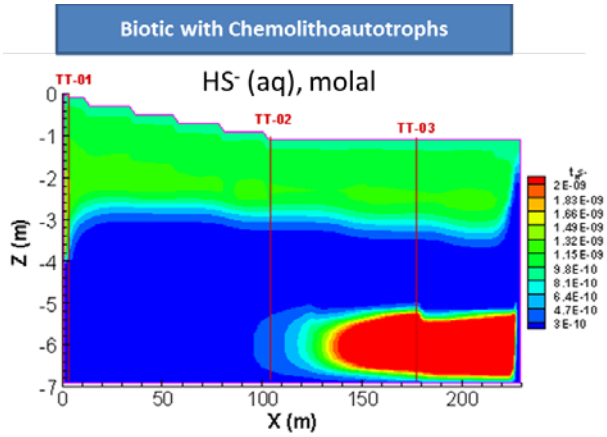
Locations of instrumented boreholes.

Tensiometers, piezometers, pore water samplers, gas samplers, and thermistors were installed in boreholes along a transect aligned with the groundwater flow direction. Hydraulic potential profiles reflect responses to precipitation, evapotranspiration, and seasonal water table variations controlled by river stage. Pore water chemical profiles exhibit elevated salinity, bicarbonate alkalinity, and organic carbon (especially within the rhizosphere). Remnants of elevated U and V from past ore milling activities persist in deeper sediments. The hydraulic and chemical data indicate that net recharge through the floodplain into the alluvial aquifer is low, seasonal, and related to microtopographic controls on precipitation runoff and ponding. Profiles of CO_2 in the vadose zone gas phase reflect strong seasonal variations in diffusive fluxes, and temperature-dependent CO_2 production and fluxes at the soil surface. These measurements of spatial and temporal distributions of subsurface chemical compositions and fluxes are improving understanding of chemical cycles within the Rifle floodplain.

Contributors: **Tetsu K. Tokunaga** and others

Modeling vertical redox zonation in the Rifle floodplain:

We are developing a 2D variably saturated reactive transport model for the Rifle Flood Plain using TOUGHREACT that couples hydrologic, biogeochemical and thermal processes to microbial functional distributions inferred from site-specific 'omic' data and applying to biogeochemical dynamics. The figure below shows that the 2D model is able to reproduce the spatially-variable redox zonation observed at the site, including the development of a bio-reduced area observed along the southern edge of the site (e.g., in the vicinity of well TT-03). This zonation is achieved by incorporating reactions for the microbial degradation of organic matter as well as contributions from chemo(litho)autotrophic microbially-mediated processes (e.g., ammonia, sulfur and iron oxidation). The importance of these pathways is supported by field scale observations of microbial distributions, along with genomic studies. The model is applied to understand the interplay of transport and biogeochemical reactions controlling carbon dynamics over time scales of a month to years.



At the Rifle site, annual temperature variations of as much as 10ºC are observed at shallow depths (< 1m), with a noticeable effect (1ºC) down to depths as much as about 7m. Groundwater fluctuations of approximately 1m have also been observed following the snowmelt recharge months. The modeling indicates that it is necessary to include seasonal water table variations and temperature fluctuations to reproduce CO2 gas concentrations observed in the vadose zone at this site.

Contributors: **Bhavna Arora** and others

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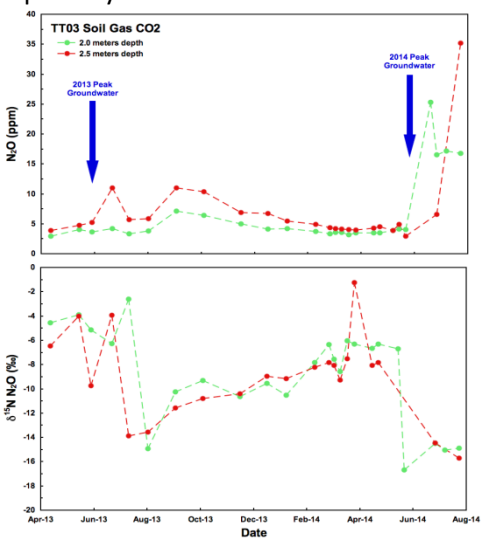
Isotopic Insights into the Fate of Porewater Nitrate:

Nitrogen isotope compositions of N2O in the unsaturated zone indicates denitrification of porewater nitrate is the primary source of N2O.



Concentrations and nitrogen isotopic compositions of N_2O in soil gas from 2.0 and 2.5 m depth in the TT03 monitoring well. Groundwater peaked at a depth of ~3 m in June 2013 and 2.25 m in June 2014.

N_2O concentrations and isotopic compositions in gas samples from the unsaturated zone at the Rifle site have been analyzed over a 15-month period (April 2013 through July 2014) to determine the source of N_2O. During this period, the groundwater level in the subsurface peaked twice during mid-June in response to high water levels in the Colorado River due to snowmelt. Following this high water episode, which was much more pronounced in 2014 than 2013, high concentrations of nitrate were observed in porewater samples collected from the lower part of the vadose zone. High concentrations of N_2O (to 10x background), a very potent greenhouse gas, were also observed in the overlying unsaturated zone. The $d^{15}N$ of the N_2O drops sharply by 10 to 12‰ then slowly increases to its background composition as the concentration decreases suggesting the primary isotopic composition of the N_2O is about -16‰. The $d^{15}N$ of soil organic matter in these sediments is ~4‰, giving a net fractionation of -20‰. This is typical of N_2O formed from denitrification of nitrate, but much lower than what is expected for other microbial sources of N_2O such as nitrification and ammonia oxidation.

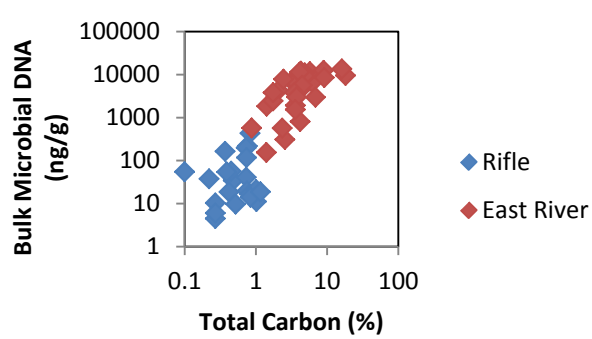
Contributors: **Mark Conrad** and others

Using Geochemical Indicators to Distinguish High Biogeochemical Activity in Sediments:

We established a relationship between total carbon and bulk microbial DNA at Rifle and East River field sites.

This study investigates geochemical parameters that can be indicators of microbial "hot spots", regions of elevated biogeochemical activity. 33 sediment samples were collected from drill cores across the Rifle floodplain along with 33 soil samples from the near surface on three meanders in the East River. DNA was extracted and quantified using a Powersoil DNA Isolation Kit and Qubit Fluorometer. Total carbon was analyzed using a coulometer. Plotting the results revealed a distinct relationship on a log plot with Rifle sediments in the lower range and East River soils in the upper range. These results support the use of carbon as a potential indicator for dense microbial populations. Further work will involve establishing the total organic carbon relationship and quantifying the percentage of the DNA which represent nitrogen and sulfate reducers respectively. Additional samples were also collected from a fourth meander in the East River to determine carbon trends across a cutoff oxbow. An oxbow will be particularly interesting in terms of the organic carbon flux because it is presumably still receiving some carbon from groundwater flow but, with an inactive channel, the contribution from overbank deposition is no longer present.

Contributors: **Amy Kenwell (CSM)** and others



Relationship between total carbon and bulk microbial DNA on Rifle and East River floodplains

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FEATURED PUBLICATIONS:

A few recent publications highlights are provided below associated with SFA 1.0 research; please visit our website to see a full list of our publications

AGU PUBLICATIONS

Water Resources Research

Bayesian hierarchical approach and geophysical data sets for estimation of reactive facies over plume scales ,by Haruko M. Wainwright, Jinsong Chen, Doug Sassen and Susan Hubbard developed a stochastic model to integrate multiscale geophysical and point data sets for characterizing coupled subsurface physiochemical properties over plume-relevant scales, which is desired for parametizing reactive transport models. They utilized the concept of reactive facies, which is based on the hypothesis that subsurface units can be identified that have distinct reactive-transport-property distributions. Read more

Environmental Science & Technology

An article entitled **Additive Surface Complexation Modeling of Uranium(VI) Adsorption onto Quartz-Sand Dominated Sediments**, by Wenming Dong and Jiamin Wan was published in Environmental Science & Technology. Their experimental results indicate that quartz has stronger U(VI) adsorption ability per unit surface areathan goethite and kaolinite at pH ≤ 4.0. Their modeling results indicate that the binary (goethite/kaolinite) CA-SCM under-predicts U(VI) adsorption to the quartz-sand dominated sediments at pH ≤ 4.0. The new ternary (quartz/goethite/kaolinite) CA-SCM provides excellent predictions. The contributions of quartz-sand, kaolinite, and goethite to U(VI) adsorption and the potential influences of dissolved Al, Si, and Fe are also discussed. Read more

Environmental Science & Technology

Bioimmobilization of Cr in Contaminated Aquifers: In studying reductive chromium immobilization Harry Beller, Peter Nico, and their colleagues found that flow-through columns constructed with homogenized aquifer sediment—and continuously infused with lactate, chromate, and various native electron acceptors—diverged to have very different Cr(VI)-reducing biogeochemical regimes, characterized by either denitrifying or fermentative conditions (as indicated by effluent chemical data, 16S rRNA pyrotag data, and metatranscriptome data). Despite the two different biogeochemical environments that evolved in the columns, these regimes created similar Cr(III)–Fe(III) hydroxide precipitates as the predominant Cr(VI) reduction product, as characterized by micro-X-ray fluorescence and micro-X-ray absorption near-edge structure analysis. Read more

national ground water association

Reducing Uranium in a Contaminated Aquifer: A team of scientists led by the Ohio State University's Paula Mouser and including ESD's Ken Williams and Phil Long recently compared two types of organic-rich sediments to better understand U release mechanisms. Sediments that were artificially primed for U removal were retrieved from an area previously biostimulated, while detrital-rich sediments were collected from a location never subject to amendment. Batch incubations demonstrated that primed sediments rapidly removed uranium from the groundwater, whereas naturally reduced sediments released a sizeable portion of U before U(VI)-reduction commenced.

These investigations stress the importance of characterizing zones with heterogeneous carbon pools at U-contaminated sites prior to the determination of a remedial strategy, to identify areas which may contribute to long-term sourcing of the contaminants. Read more

SFA 2.0 EARLY CAREER SPOTLIGHT: BAPTISTE DAFFLON

Baptiste Dafflon started his career at Lawrence Berkeley Lab's Earth Sciences as a Postdoc in 2011. He has since advanced to a Project Scientist. He received his Ph.D. in geophysics from the University of Lausanne (Switzerland). Then, he obtained a Swiss National Science Foundation postdoc fellowship to pursue his research in hydrogeophysics at the Center of Geophysical Investigation of the Shallow Subsurface (CGISS) at Boise State University. Baptiste has been awarded the 2013 Paul Niggli Medal for his "original research contributions to the geophysical exploration of aquifers and permafrost environments".

Baptiste's research interests are the inherently trans-disciplinary fields of environmental geophysics, hydrology and biochemistry. Currently his research focuses primarily on the development of comprehensive strategies for advanced monitoring of landscape and soil properties across spatial scales (including geophysical data, point-scale measurements, and remote sensing information), and on the integration and inversion of multiple sources of geophysical and hydrological information to improve the prediction and understanding of coupled subsurface processes

His research in SFA 2.0 focuses on estimating hydraulic and thermal properties using geophysical and hydrological data, inferring high-resolution digital surface elevation model and multi-spectral images (kite- and UAV- based), and investigating interactions between landscape and subsurface properties (spatially and temporally).

On a personal note, Baptiste always enjoys outdoor activities, including geophysical data acquisition campaigns, hiking and backpacking in the Sierra Nevada with his family, and tasting beers with friends on a terrace.

AWARDS and ACHIEVEMENTS:

Susan Hubbard elected as a 2014 member to the University of California Berkeley Civil and Environmental Engineering (CEE) Department Academy of Distinguished Alumni.

Boris Faybisheko appointed Editorial Board Member, Senior Editor (Environmental Science) of the Oxford Research Encyclopedia of Environmental Science of Oxford University Press.

SFA 2.0 KEY COLLABORATORS:

The SFA 2.0 is sponsored by the U.S. Department of Energy, Biological, and Environmental Research, Subsurface Biogeochemical Research Program.
David Lesmes, Program Manager, can be reached at David.Lesmes@science.doe.gov

QUESTIONS/COMMENTS:

Send any comments or questions concerning this newsletter to:

Lisa M. Kelly, lmkelly@lbl.gov