Monitoring of nitrous oxide emissions during soil drying with X-ray computed tomography

Eva Rabot, Marine Lacoste, Isabelle I. Cousin, Catherine Hénault

Complex Soil Systems 2014

A Path to Improved Understanding of Complex Soil Systems

David Brower Center • Berkeley, California • September 3–5, 2014

Soil Science Society of America
Berkeley Lab
ESD Earth Sciences Division
Subsurface Biogeochemical Research
Department of Energy United States of America
Terragenome
Vadose Zone Journal
MO BIO Laboratories, Inc.
AGU American Geophysical Union
Environmental Services Association of Alberta ESAA

Proceedings of the Complex Soil Systems Conference

"A Path to Improved Understanding of Complex Soil Systems"

Supported by SSSA/Bouyoucos Funds, Berkeley Lab, and DOE

Abstracts

September 3 – 5, 2014

David Brower Center
Berkeley, California

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Foreword

Soils are complex systems that are host to a variety of interactions between physical, geochemical and biological processes. This flagship conference will make a unique contribution to integrated soil sciences by addressing fundamentals and bridging gaps in the current scientific knowledge. A goal is to provide a motivating framework to a path towards improved understanding of complex soil systems. The conference is intended to provide a forum for in-depth group discussions, for soliciting feedback on emerging concepts and engaging colleagues with similar interests of the emerging questions:

- What are the recent advances in fundamental, experimental, and modeling studies of how soil physical, chemical and biological processes interact to control terrestrial C and N cycles and water resource sustainability?
- How can we take advantage of recent advances in biogeochemistry, genomics, multi-scale imaging and computational and mathematical methods for diagnosing nonlinear dynamical processes and complexity, to study emergence of new behaviors or functions as scale changes from the nanoscale to microscopic, mesoscopic, and macroscopic field levels?
- Can we quantify plant-soil feedbacks, complexity, uncertainty, and nonlinear dynamical and chaotic processes in complex soil systems to improve predictions in managed and unmanaged ecosystems with application to agriculture, remediation, and carbon sequestration?

More than 120 abstracts were submitted from microbiologists, ecologists, biogeochemists, soil physicists, agricultural scientists, hydrologists, geophysicists, climatologists, and others working on key aspects of complex soil systems in 12 countries.

The following themes will be discussed during the conference with panel discussions following each theme to provide opportunities for collaborative synthesis of key topics.

Theme 1: Complex Soil Systems: Fundamental concepts of how soil physical, chemical and biological components and processes influence the soil-plant-atmosphere system at multiple spatial and temporal scales.

Theme 2: Advanced In-Situ Soil Characterization and Experimentation: Quantification of critical in-situ soil processes using genomic, synchrotron, isotopic and field biogeophysical techniques.

Theme 3: Modeling of Soil Systems: Conceptual, theoretical, and numerical models to describe and predict soil systems behavior - linear and nonlinear dynamical models, stochastic, deterministic, and deterministic-chaotic modeling approaches, self-organizing and emergent processes.

Theme 4: Soil Systems and Global Climate Change: Integrated observations, models, and case studies that document how soils are affected by and also influence global climate change at spatial and temporal scales.

Theme 5: Using a Complex System Approach for Practical Applications: Theory and case studies from managed and unmanaged systems (agriculture, irrigation, remediation, natural ecosystems, carbon sequestration, etc.)

Theme 6: Defining and Visualizing Complexity Across Scales.

Theme 7: Moving Forward **-** Research Coordination, Building the Ecosystem.

Additional updated information including any changes to the Program will also be available on the website.

The Organizing Committee wishes to thank in advance the session chairs, presenters, invited speakers, and participants for their participation in our Complex Soil Systems Conference. We also are grateful to all our sponsors: Earth Sciences Division at Lawrence Berkeley National Laboratory, Mo Bio Laboratories Inc., Soil Science Society of America, U.S. Department of Energy Subsurface Biogeochemical Research program, The PRIME Program in the Life Sciences Division at Berkeley Lab the TerraGenome consortium, private donors, American Geophysical Union, Environmental Services Association of Alberta, and the Vadose Zone Journal.

The Organizing Committee

Berkeley, CA, September 2014

SSSA/BOUYOUCOS FUNDS AND BERKELEY LAB "COMPLEX SOIL SYSTEMS" CONFERENCE

SEPTEMBER 3-5, 2014

Complex Soil Systems Conference
"A Path to Improved Understanding of Complex Soil Systems"
David Brower Center
Berkeley, California

Time	Title	Room
	Tuesday, September 2, 2014	
	Icebreaker	
6:00 PM	**Welcome Reception** *Including a presentation on the Concept of Complexity by Fred Molz*	Hotel Shattuck Plaza
	Wednesday, September 3, 2014	
7:30 AM	**Registration**	David Brower Center
	Welcome and Opening Remarks	
8:30 AM	**Welcome** **Susan Hubbard,** Earth Sciences Division Director, Lawrence Berkeley National Laboratory (LBNL)	Goldman Theater
8:40 AM	**Opening Remarks** **Jan W. Hopmans,** University of California, Davis; Soil Science Society of America President	
8:55 AM	**Announcements** **Complex Soil Systems Organizing Committee**	
	Theme 1: Complex Soil Systems – Fundamental Concepts	
	Session Chairs: Eoin Brodie, Mark Williams	
9:00 AM	**A theory of soil?** **John W. Crawford** (Rothamsted Research, UK) *invited*	Goldman Theater
9:30 AM	**A new worldview of soils** **Henry Lin** (Penn State University)	
9:50 AM	**Motility in water films and trophic interactions shape self-organization of microbial consortia on hydrated soil surfaces** **Dani Or,** Gang Wang, Robin Tecon (Swiss Federal Institute of Technology Zurich) *invited*	
10:10 AM	**Peat: A complex soil with dual-porosity media** **Fereidoun Rezanezhad** and Philippe Van Cappellen (University of Waterloo, Canada)	
10:30 AM	*Break*	Gallery

Time	Title	Room
10:50 AM	**Mucilage: the hydraulic bridge between roots and soil** **Andrea Carminati**, M. Zarebanadkouki, E. Kroener, M. Ahmed (University of Goettingen, Germany)	Goldman Theater
11:10 AM	**Geochemical and microbiological complexity in soil-sediment redox oscillations** **Eric Roden** (University of Wisconsin-Madison)	
11:30 AM	**Panarchy in soil systems: Towards evaluating resilience across multiple spatial scales** **Morgan M. Williams** (University of California, Berkeley)	
11:50 AM	*Lunch*	Gallery/ Terrace

Theme 2: Advanced In-Situ Soil Characterization and Experimentation

Session Chairs: Peter Nico, Janet Jansson

Time	Title	Room
1:00 PM	**Complexity in soil biogeochemical processes arising from aggregate-scale heterogeneity** **Scott Fendorf**, Marco Keiluweit (Stanford University), Markus Kleber (Oregon State University), Peter Nico (LBNL) ***invited***	Goldman Theater
1:30 PM	**Mass spectrometry approaches for analysis of soil organic matter composition and bacterial cycling** Richard Baran, Tami L. Swenson, Nicholas Justice, Ulas Karaoz, Romy Chakraborty, Stefan Jenkins, R. Lau, Benjamin Bowen, Adam Arkin, Adam Deutschbauer, Eoin L. Brodie, **Trent Northen** (LBNL)	
1:50 PM	**Unearthing complex soil microbial communities using omics** **Janet Jansson** (Pacific Northwest National Laboratory, PNNL) *invited*	
2:10 PM	**Advanced characterization of soil organic matter using ultra high resolution mass spectrometry** Malak M. Tfaily, Rosey Chu, Nikola Tolić, **Kristyn M. Roscioli**, Errol R. Robinson, Ljiljana Paša-Tolić, Nancy J. Hess (PNNL)	
2:30 PM	**Advanced *in-situ* measurement of soil carbon content using inelastic neutron scattering** **Galina Yakubova**, Alexander Kavetskiy, H. Allen Torbert, Stephen A. Prior (USDA-ARS National Soil Dynamics Laboratory)	
2:50 PM	**Geophysical identification and characterization of permafrost soil functional zones** **Susan S. Hubbard**, Haruko Wainwright, Baptiste Dafflon (LBNL), Janet Jansson (PNNL), Tim Kneafsey, Neslihan Tas, Yuxin Wu, Margaret Torn (LBNL)	
3:10 PM	**Moving away from the geostatistical lamppost: Why, where, and how does the spatial heterogeneity of soils matter?** **Philippe C. Baveye** (Rensselaer Polytechnic Institute) and Magdeline Laba (Cornell University)	
3:30 PM	*Break*	Gallery

Time	Title	Room
Theme 3: Modeling of Soil Systems		
Session Chairs: Fred Molz, Yakov Pachepsky		
3:50 PM	**Complexity, chaotic dynamics and mathematical modeling** **Fred Molz** (Clemson University) and Boris Faybishenko (LBNL)	Goldman Theater
4:10 PM	**Saturation dependence of transport in soils: Modern theories** **Allen G. Hunt** and Behzad Ghanbarian (Wright State University, Dayton) ***invited***	
4:30 PM	**Thermodynamics and pedogenesis differences between desert microsites** **Michael H. Young**, T.G. Caldwell (University of Texas at Austin), H. Lin (Pennsylvania State University)	
4:50 PM	**Mineral interactions, microbial processes, and transport explain long residence times of rapidly decomposable deep soil organic matter** **William J. Riley**, Margaret S. Torn, Jinyun Tang, Dipankar Dwivedi (LBNL), Federico M. Maggi (The University of Sydney), Markus Kleber (Oregon State University)	
5:10 PM	**A bioenergetic approach to constrain substrate quality in carbon turnover models** **Douglas E. LaRowe** (University of Southern California), Bill Riley (LBNL), David D. Myrold, Markus Kleber (Oregon State University), Jinyun Tang (LBNL)	
5:30 PM	**The kinematics of root-soil interactions** **Wendy Silk** (University of California, Davis) and Lionel X. Dupuy (University of California, Davis; The James Hutton Institute, Invergowrie Dundee)	
Evening Poster Session and Reception		
6:00 – 8:00	Poster Session and Reception	Kinzie & Tamalpais
Thursday, September 4, 2014		
Theme 4: Soil Systems and Global Climate Change		
Session Chairs: Charles Koven, Bill Riley		
8:30 AM	**The microbial ecology of soil carbon** **Bruce Hungate** (NAU) ***invited***	Goldman Theater
9:00 AM	**Bridging soil physics and ecosystem ecology towards better understanding soil trace gas efflux** **Dennis Baldocchi** (University of California, Berkeley) ***invited***	
9:20 AM	**Microbes as the living component of complex soil systems: Data and models** **Xiaofeng Xu** and Peter E. Thornton (Oak Ridge National Laboratory, ORNL)	
9:40 AM	**The effect of a warmer climate on soil carbon cycling: Emergent responses across time and space scales** **Jennifer Harden** (U.S. Geological Survey, emeritus) and Margaret Torn (LBNL) ***invited***	
10:00 AM	*Break*	Gallery
10:20 AM	**Climate-change effects on inorganic and organic carbon cycling in soils** **Nik Qafoku** (PNNL)	Goldman

Time	Title	Room
10:40 AM	**Hydromechanics of high elevation meadows: Resiliency and thresholds of complex soils** **Teamrat A. Ghezzehei**, Chelsea L. Arnold, Asmeret Asefaw Berhe (University of California, Merced)	Theater
11:00 AM	**Mesoscale soil-surface heterogeneity as a controlling influence on the generation of macropore flow** **John R. Nimmo** (U.S. Geological Survey)	
11:20 AM	**Capturing transient climate-driven contributions of surface to subsurface processes at watershed scales** **David Watson**, Scott Brooks, Guoping Tang, Chris Schadt, Nathan Collier, Jennifer Earles, Tonia Mehlhorn, Kenneth Lowe (ORNL), Pengsong Li (Peking University), Fengming Yuan (ORNL)	
11:40 AM	Panel Discussion *(lead by Session Chairs)*	
12:10 PM	*Lunch*	Gallery/ Terrace

Theme 5: Using a Complex System Approach for Practical Applications

Session Chairs: Margaret Torn, Ron Amundson

Time	Title	Room
1:40 PM	**Nurturing the link between resilience, complexity and sustainability at the landscape scale** **Lael Parrott** (Okanagan Institute for Biodiversity, Resilience, and Ecosystem Services (BRAES), The University of British Columbia, Okanagan Campus, Kelowna, BC) *invited*	Goldman Theater
2:10 PM	**Practical application of chaotic advection to groundwater remediation** **David C. Mays**, Matt N. Jones (University of Colorado, Denver), Roseanna M. Neupauer (University of Colorado, Boulder)	
2:30 PM	**Soil water content variability in the 3D 'support-spacing-extent' space of scale metrics** **Yakov Pachepsky** (USDA-ARS Beltsville Agricultural Research Center), Harry Vereecken (Institute of Agrosphere, Research Center Jülich, Germany), Gonzalo Martinez Garcia (The Institute for Agricultural and Fisheries Research and Training, Spain)	
2:50 PM	**Modelling the optimal phosphate fertiliser and soil management strategy for crops** **James Heppell,** S. Payvand (University of Southampton, UK), P. Talboys (University of Bangor, UK), K. Zygalakis, J. Fliege (University of Southampton, UK), R. Sylvester-Bradley (ADAS, Boxworth, Cambridge), R. Walker (Scotland's Rural College, Craibstone Estate), D.L. Jones (University of Bangor, UK), T. Roose (University of Southampton, UK)	
3:10 PM	**Soil salinity measurement and habitat sustainability in brackish seasonally managed wetlands** **Nigel W.T. Quinn** (LBNL)	
3:30 PM	*Break*	Gallery
3:50 PM	**Latent approaches to linking "omics" with belowground processes: a methane case study** **Jason Barker**, J. Christiansen, S. Grayston (University of British Columbia)	Goldman Theater

Time	Title	Room
4:10 PM	**Rethinking nutrient limitation in soils: Linking soil carbon cycling to phosphorus availability with Biological Stoichiometry Theory** **Wyatt H. Hartman** (DOE Joint Genome Institute), C. Richardson (Duke University), Susannah Tringe (DOE Joint Genome Institute)	
4:30 PM	Panel Discussion *(lead by Session Chairs)*	

Evening Poster Session and Reception

5:30 – 8:00	Poster Session and Reception	Kinzie & Tamalpais

Friday, September 5, 2014

Theme 6: Defining and Visualizing Complexity Across Scales

Session Chairs: Deborah Agarwal, Nicholas Bouskill

8:30 AM	**Remote sensing of belowground variation in trembling aspen forests** **Michael D. Madritch** (Appalachian State University), Clayton C. Kingdon, Aditya Singh (University of Wisconsin, Madison), Karen E. Mock (Utah State University), Richard L. Lindroth, Philip A Townsend (University of Wisconsin, Madison) ***invited***	Goldman Theater
8:50 AM	**Soil landscape systems: A scalar framework for modeling soil processes and properties** Doug Wysocki, **Philip Schoeneberger**, Zamir Libohova (USDA-NRCS-National Soil Survey Center)	
9:10 AM	**Measuring and scaling dynamic soil properties in soil survey** **Skye Wills**, Candiss Williams, Philip Schoeneberger, Doug Wysocki, Zamir Libohova, Cathy Seybold (USDA-NRCS-National Soil Survey Center)	
9:30 AM	**MultiScale visualization of complex subsurface processes** **Harinarayan Krishnan** (LBNL)	
9:50 AM	Panel Discussion *(lead by Session Chairs)*	
10:20 AM	*Break*	Gallery

Theme 7: Moving Forward - Research Coordination, Building the Ecosystem

Session Chairs: Susan Hubbard, Wendy Silk

10:40 AM	International soil experiment network **Margaret Torn** (LBNL) and Jennifer Harden (U.S. Geological Survey, emeritus)	Goldman Theater
11:00 AM	**On the need to establish an international soil modeling consortium** **Harry Vereecken et al.** *(multiple authors and organizations – please see abstract for a complete list)*	
11:20 AM	**Data coordination for multiscale complex systems analysis** **Deborah Agarwal** (LBNL)	
11:40 AM	"Panel Discussion Session" on the future directions and international efforts **Moderator: Peter Nico** **Panel:** Ronald Amundson, Eoin Brodie, John Crawford, Scott Fendorf, John Nimmo, Dani Or, Margaret Torn, Harry Vereecken	
12:30 PM	**Closing Remarks / Adjourn**	

POSTER SESSION I

Wednesday, September 3rd, 6:00 – 8:00 PM
David Brower Center

Board	Title/Author
Theme 1: Complex Soil Systems – Fundamental Concepts	
Kinzie Room (*1st floor*)	
Board 1	**Influence of soil bacteria on nitrogen uptake and transfer by arbuscular mycorrhizal fungi** **Rachel Hestrin** and Johannes Lehmann (Cornell University)
Board 2	**Acid phosphatase activity in the rhizosphere: how a cereal and a legume create local hotspots** **Sarah Placella**, Gabrielle Daudin (Montpellier SupAgro-CIRAD-INRA-IRD), Naoise Nunan (CNRS, BioEMCo, Campus AgroParisTech), Esther Guillot, Josiane Abadie, Camille Gros, Claire Marsden, Philippe Hinsinger (Montpellier SupAgro-CIRAD-INRA-IRD)
Board 3	**Soil chronosequence elucidates development of soil structure heterogeneity** **Marjorie Schulz**, Corey Lawrence, Jane Manning, Dave Stonestrom (U.S. Geological Survey)
Board 4	**Soil microbial heterogeneity at the micrometer scale** **Neslihan Tas**, Giovanni Birarda, Marco Voltolini, Shi Wang, Hoi-Ying Holman, Jonathan Ajo-Franklin (Lawrence Berkeley National Laboratory, LBNL), Janet Jansson (Pacific Northwest National Laboratory, PNNL), Eoin L. Brodie (LBNL)
Theme 2: Advanced In-Situ Soil Characterization and Experimentation	
Tamalpais Room (*2nd floor*)	
Board 14	**Probing microbial territorial disputes using advanced correlative imaging technologies** **Manfred Auer** (LBNL)
Board 15	**Mapping potential metabolic interactions among soil bacteria using exometabolomics** **Richard Baran**, Benjamin P. Bowen, Megan A. Danielewicz, Tami Swenson, Stefan Jenkins, Romy Chakraborty, Ulisses Nunes Da Rocha, Eoin L. Brodie (LBNL), Jazmine Mayberry-Lewis, Hinsby Cadillo-Quiroz, Ferran Garcia-Pichel (Arizona State University), Adam P. Arkin, Adam M. Deutschbauer, Trent R. Northen (LBNL)
Board 16	**Assessment of soil bacterial diversity patterns in Mediterranean Ecosystems of Crete (Eastern Mediterranean Basin)** **Fotios Bekris** (University of Crete, Heraklion, Greece; LBNL), Lauren Tom, Yvette Piceno (LBNL), Nickolas Panopoulos (University of Crete, Heraklion and Rethymno, Greece), Gary Andersen (LBNL), Stergios Pirintsos (University of Crete, Heraklion and Rethymno, Greece)
Board 17	**Tracking the temporal dynamics of cellulose utilization by bacteria and fungi in soil using ^{13}C-stable isotope probing and next generation sequencing** **Ashley Campbell**, Charles Pepe-Ranney, Chantal Koechli, Sean T. Berthrong, Daniel H. Buckley (Cornell University)
Board 18	**Experimental studies of ambient-level noble gas dynamics in porous media: fractionation and evaluation of transport mechanisms through advective-diffusive and dusty-gas models** **Xin Ding**, Mack B. Kennedy (LBNL), William C. Evans, David A. Stonestrom (U.S. Geological Survey)

Board	Title/Author
Board 19	Microbial community dynamics in salt crusts of the hyperarid Atacama Desert **Kari Finstad** (University of California, Berkeley), Yvette Piceno, Gary Andersen (LBNL), Ronald Amundson (University of California, Berkeley)
Board 20	Autonomous millimeter-Scale RFID Sensors for High Density *In-Situ* Soil Monitoring **Erin G. Fong**, Carl Grace, Peter Denes (LBNL)
Board 21	Biological stability of soil organic matter is related to thermal and chemical properties **Adam W. Gillespie** (Canadian Light Source), H. Sanei (Geological Survey of Canada), A. Diochon (Lakehead University, Ontario), C. Tarnocai (Agriculture and Agri-Food Canada (AAFC), Science and Technology Branch (STB), Ottawa, Ontario), H.H. Janzen (AAFC-STB, Lethbridge, Alberta), T.Z. Regier, D. Chevrier, J.J. Dynes (Canadian Light Source) E.G. Gregorich (Agriculture and Agri-Food Canada (AAFC), Science and Technology Branch (STB), Ottawa, Ontario)
Board 22	Bulk carbon K-edge x-ray absorption spectroscopy: Overcoming technical challenges **Adam W. Gillespie**, James J. Dynes, Tom Z. Regier, David Chevrier, Teak D. Boyko (Canadian Light Source), Derek Peak (University of Saskatchewan, Saskatoon)
Board 23	Sequential selective dissolution to quantify storage and stability of organic carbon associated with different mineral types **Katherine Heckman** (USDA Forest Service, Northern Research Station), Corey Lawrence, Jennifer Harden (U.S. Geological Survey)
Board 24	Meta- and isolate- genomics for characterization of grassland soil microbial communities **Ulas Karaoz**, Heejung Cho, Ulisses Nunes da Rocha, Eoin L. Brodie (LBNL)
Board 25	Monte-Carlo simulation of soil carbon measurements by inelastic neutron scattering **Alexander Kavetskiy**, Galina Yakubova, Stephen A. Prior, H. Allen Torbert (USDA-ARS National Soil Dynamics Laboratory)
Board 26	Synchrotron-based characterization at the APS to determine physical and chemical characteristics of carbon in the subsurface and root zones to improve Earth system modeling of the biogeochemical cycling of carbon **Ken Kemner** (Argonne National Laboratory, ANL), B. Mishra (ANL; Illinois Institute of Technology), E.J. O'Loughlin, M.I. Boyanov, S. O'Brien (ANL), V. Bailey, A. Konopka (PNNL)
Board 27	Current understanding and future directions: The form and function of the organo-mineral interface **Melanie A. Mayes**, Sindhu Jagadamma (Research Accelerator Division), Haile Ambaye (Research Accelerator Division), Loukas Petridis (Center for Molecular Biophysics), Valeria Lauter (Oak Ridge National Laboratory , ORNL), S. Michael Kilbey II (University of Tennessee, Knoxville)
Board 28	Carbon chemistry in unaltered soil samples using non-resonant inelastic x-ray scattering **Bhoopesh Mishra** (Illinois Institute of Technology, Chicago; ANL), Edward J. O'Loughlin (ANL), William T. Cooper (Florida State University), Julie Jastrow, Robert Gordon, Mahalingam Balasubramanian, Kenneth M. Kemner (ANL)
Board 29	Belowground linkages during ecosystem development: patterns of microbial community and organic matter change associated with pedogenesis J. Moon, R. Pineda, **Mark A. Williams**, K. Xia, L. Ma (Virginia Polytechnic & State University)
Board 30	A novel nanoparticle approach for imaging soil bacteria **Sarah L. O'Brien** (ANL), Matthew D. Whiteside (University of British Columbia, Okanagan), Deirdre Sholto-Douglas, Dionysios A. Antonopoulos, Maxim I. Boyanov (ANL), Daniel M. Durall, Melanie D. Jones (University of British Columbia, Okanagan), Barry Lai, Edward J. O'Loughlin, Kenneth M. Kemner (ANL)
Board 31	LBNL radiotracer and imaging technologies for microbial systems research **James P. O'Neil**, Nicholas T. Vandehey, Ross Boutchko, Mustafa Janabi, William W. Moses (LBNL), Eoin L. Brodie (LBNL; University of California, Berkeley), Peter S. Nico (LBNL)
Board 32	Visualizing the soil carbon-mineral interface: STEM-EELS analysis of soil microaggregates **Angela Possinger**, A. Enders, B. Levi, D. Muller, J. Lehmann (Cornell University)

Board	Title/Author
Board 33	**Management effect on soil organic matter distribution near intra-aggregate pore aggregate structure as determined by µCT images** **Michelle Quigley**, Alexandra Kravchenko (Michigan State University), Mark Rivers (The University of Chicago)
Board 34	**Monitoring of nitrous oxide emissions during soil drying with x-ray computed tomography** E. Rabot, **Marine Lacoste**, I. Cousin, C. Hénault (INRA)
Board 35	**Soil microbial community shifts in response to soil thermal insulation and vegetation change in moist acidic tundra of Northern Alaska** **Michael P. Ricketts**, Rachel S. Poretsky (University of Illinois, Chicago), Jeffrey M. Welker (University of Alaska, Anchorage), Miquel Gonzalez-Meler (University of Illinois, Chicago)
Board 36	**Plant invasions are associated with changes in root-zone fungal communities** **Richard R. Rodrigues**, Rosana P. Pineda, John E. Barrett, Jacob N. Barney, Eric T. Nilsen, Mark A. Williams (Virginia Polytechnic & State University)
Board 37	**Long-term and high frequency non-destructive monitoring of soil water stable isotope compositions in the laboratory** **Youri Rothfuss**, Steffen Merz, Andreas Pohlmeier, Harry Vereecken, Nicolas Brüggemann (Agrosphere Institute (IBG-3), Leo-Brandt-Straße, Germany)
Board 38	**The effect of compost on carbon cycling and the active soil microbiota** **Esther Singer**, Rebecca Ryals, Whendee Silver, Tanja Woyke (LBNL)
Board 39	**Metabolomics approaches to understand microbial carbon cycling in grassland soil** **Tami L. Swenson**, Stefan Jenkins, Benjamin Bowen (LBNL), Jillian F. Banfield (University of California, Berkeley), Trent R. Northen (LBNL)
Board 40	**Noninvasive imaging of CO_2 uptake in biological soil crusts** **Nicholas Vandehey**, Trent R. Northen (LBNL), Eoin L. Brodie (LBNL; University of California, Berkeley), Peter S. Nico, James P. O'Neil (LBNL)
Board 41	**3D characterization of soil aggregates: new opportunities from sub-micron resolution synchrotron x-ray microtomography** **Marco Voltolini**, Jonathan B. Ajo-Franklin, Neslihan Taş, Shi Wang (LBNL), Eoin L. Brodie (LBNL; University of California, Berkeley)
Board 42	**Reactive transport modeling parameterization using geophysical datasets** **Haruko M. Wainwright**, Adrian Flores-Orozco, Matthias Bücker, Baptiste Dafflon, Kenneth H. Williams, Susan S. Hubbard (LBNL)
Board 43	**Nitrogen cycling and soil fungal communities along gradients of forest composition factors and age in regenerating tropical dry forests** Bonnie G. Waring (University of Minnesota, St. Paul), **Rachel I. Adams**, Sara Branco (University of California, Berkeley), Jennifer S. Powers (University of Minnesota, St. Paul)

Theme 3: Modeling of Soil Systems

Kinzie Room (*1st floor*)

Board	Title/Author
Board 5	**Why is there universality in saturation-dependent transport?** Robert P. Ewing (Iowa State University), **Allen G. Hunt**, Behzad Ghanbarian (Wright State University)
Board 6	**Effective Permeability in Multi-Component Porous Media: Lattice-Boltzmann Model and Effective Medium Approach Applications** **Behzad Ghanbarian** (Wright State University, Dayton) and Hugh Daigle (University of Texas at Austin)
Board 7	**Theoretical relationship between surface fractal dimension and water content measured at permanent wilting point: adsorbed water films effect** **Behzad Ghanbarian** (Wright State University) and Humberto Millán (University of Granma)
Board 8	**FLOGing data to link carbon and nitrogen cycling from organic matter additions to agroecosystems** **J. Daniel Gillis** (McGill University) and Gordon W. Price (Dalhousie University)

Board	Title/Author
Board 9	**Trait-based approaches to modeling microbial biogeochemistry from terrestrial to aquatic ecosystems** **Eric King**, Sergi Molins, Ulas Karaoz, Nicholas J. Bouskill (LBNL), L.A. Hug, B.C. Thomas, C.J. Castelle (University of California, Berkeley), Harry R. Beller (LBNL), Jill F. Banfield (University of California, Berkeley), Carl I. Steefel, Eoin L. Brodie (LBNL)
Board 10	**Reduced-order modeling of fine-resolution hydrologic and biogeochemical simulations at NGEE-Arctic study sites** **Yaning Liu**, George Shu Heng Pau, Gautam Bisht, Williams Riley (LBNL)
Board 11	**Self-organization, emergence, and fractal dimension of colloid deposits in model soils** **David C. Mays**, Eric J. Roth (University of Colorado, Denver), Benjamin Gilbert (LBNL)
Board 12	**A zero-sum-game-based model for litter decomposition dynamics** **Jinyun Tang** and William J. Riley (LBNL)
Board 13	**Modeling microbial degradation of soil organic matter with a genome scale metabolic reconstruction of Hopland isolates** **Kateryna Zhalnina**, Stefan Jenkins, Ulas Karaoz (LBNL), Shengjing Shi, Heejung Cho (University of California, Berkeley), Nicholas Bouskill, Trent R. Northen (LBNL), Mary K. Firestone, Eoin L. Brodie (University of California, Berkeley; LBNL)

POSTER SESSION II

Thursday, September 4th, 5:30–8:00 PM
David Brower Center

Board	Title/Author
Theme 4: Soil Systems and Global Climate Change	
Kinzie Room (*1st floor*)	
Board 1	Predicting soil bacterial responses to multi-factor global change with trait-based Modeling **Nicholas J. Bouskill** (LBNL), Xavier Le Roux (INRA, CNRS, Université Lyon), Jinyun Tang (LBNL)
Board 2	A trait-based model for understanding rates, patterns, and ecological consequences of microbial nitrogen fixation in high-latitude terrestrial ecosystems **Yiwei Cheng**, William Riley, Jinyun Tang, Nicholas Bouskill (LBNL)
Board 3	The pulsed response of soil respiration to precipitation in an African savanna ecosystem: A coupled measurement and modeling approach **Zhaosheng Fan** (ANL), Jason C. Neff (University of Colorado, Boulder), Niall P. Hanan (South Dakota State University)
Board 4	Interconnections among aggregate structures, organic matter, and microbes in rhizosphere-dominated soils Julie Jastrow, R. Michael Miller, Sarah L. O'Brien, **Roser Matamala** (ANL)
Board 5	Permafrost carbon-climate feedback: Sensitivity to deep soil decomposability and nitrogen cycle **Charles D. Koven** (LBNL), D.M. Lawrence (National Center for Atmospheric Research, Boulder), W.J. Riley (LBNL)
Board 6	Non-linear response of soil carbon gas (CO_2, CH_4) flux to oxygen availability **Gavin McNicol** and Whendee L. Silver (University of California, Berkeley)
Board 7	Biogeochemistry of the microbial soil sink of carbonyl sulfide (COS) - a carbon cycle tracer **Laura K. Meredith,** Paula V. Welander (Stanford University), Joe Berry (Carnegie Institution for Science)
Board 8	Classifying visual quality assessment of time series data into data quality patterns **Gilberto Pastorello** (LBNL), Dario Papale (University of Tuscia), Deb Agarwal (LBNL), Carlo Trotta (University of Tuscia), Cristina Poindexter, Boris Faybishenko (LBNL), Eleonora Canfora (euroMediterranean Center on Climate Change), Taghrid Samak, Dan Gunter (LBNL), Alessio Ribeca (University of Tuscia), Rachel Hollowgrass (LBNL)
Board 9	The role of hydrodynamic methane transport in soil-atmosphere methane fluxes in a temperate marsh **Cristina M. Poindexter** (University of California, Berkeley), Emily Gilson (Princeton University), Sara H. Knox (University of California, Berkeley), Jaclyn Hatala Matthes (Dartmouth College), Joseph G. Verfaillie, Dennis D. Baldocchi, Evan A. Variano (University of California, Berkeley)
Board 10	Assessing kinetics of Fe reduction and degradation of organic matter in subalpine wetland soils **Kathrin Schilling** and Céline Pallud (University of California, Berkeley)
Board 11	Physical and biological processes interact to determine soil carbonyl sulfide uptake in two contrasting ecosystems Ulli Seibt, **Wu Sun** (University of California, Los Angeles), Sabrina Juarez, Kadmiel Maseyk, Céline Lett (Bioemco, University Pierre & Marie Curie)

Board	Title/Author
Board 12	Resolving terrestrial ecosystem processes along a subgrid topographic gradient for an earth-system model **Zachary M. Subin** (Princeton University; National Oceanic and Atmospheric Administration; U.S. Geological Survey), P.C.D. Milly (U.S. Geological Survey; National Oceanic and Atmospheric Administration), B.N. Sulman (National Oceanic and Atmospheric Administration; Indiana University), S. Malyshev, E. Shevliakova (Princeton University; National Oceanic and Atmospheric Administration)
Board 13	Microbial ecology across polygon types and features at the NGEE-Arctic Barrow site **Neslihan Tas**, Shi Wang, Yuxin Wu, Lydia Smith, Craig Ulrich, Timothy Kneafsey, Margaret Torn, Susan S. Hubbard (LBNL), Janet K. Jansson (PNNL)

Theme 5: Using a Complex System Approach for Practical Applications

Tamalpais Room (2nd *floor*)

Board	Title/Author
Board 14	Willow growth and bioaccumulation of contaminant metals: links with dominant ectomycorrhizal fungi **Terrence H. Bell et al.** *(multiple authors and organizations – please see abstract for a complete list)*
Board 15	Increased crop yields and differing soil properties as a result of two native woody shrubs in the Peanut Basin, Senegal **Nathaniel A. Bogie** (University of California, Merced)**,** R. Bayala, I. Diedhiou (University of Thies, Senegal; Institut Senegalais de Recherche Agricole (ISRA)), T.A. Ghezzehei (University of California, Merced), R. Dick (Ohio State University)
Board 16	Amendment effects on arsenic uptake in paddy rice – deciphering the regulating mechanisms **Kristin Boye** (Stanford University), A.M. Herrmann (Swedish University of Agricultural Sciences, Sweden), M.V. Schaefe, S. Fendorf (Stanford University)
Board 17	The implications of soil moisture spatial scaling structure for sampling of the soil moisture field **Jingnuo Dong** and Tyson E. Ochsner (Oklahoma State University, Stillwater)
Board 18	The impact of winter cover crop development on nitrate leaching: combining field observations with computer modeling **Matthew R. Dumlao**, Ahmad B. Moradi, Martin Burger, Jan W. Hopmans, William R. Horwath, Wesley W. Wallender, Wendy K. Silk (University of California, Davis)
Board 19	Influence of diesel contamination in soil on the growth and dry matter partitioning of lactuca sativa and ipomoea batata **Kayode Fatokun** and G.E. Zharare (University of Zululand, Kwa-Dlangezwa)
Board 20	Hierarchical clustering and principal component analysis as tools for classification and selecting representative field sites **Boris Faybishenko**, Susan S. Hubbard, Philip Long, Kenneth H. Williams (LBNL)
Board 21	Modelling the optimal phosphate fertiliser and soil management strategy for crops **James Heppell**, S. Payvand (University of Southampton, UK), P. Talboys (University of Bangor, UK), K. Zygalakis, J. Fliege (University of Southampton, UK), R. Sylvester-Bradley (ADAS, Boxworth, Cambridge), R. Walker (Scotland's Rural College, Craibstone Estate), D.L. Jones (University of Bangor, UK), T. Roose (University of Southampton, UK)
Board 22	Predicting saturated hydraulic conductivity by soil parametric and morphological properties **Gülay Karahan** and Sabit Ersahin (Cankırı Karatekin University, Cankırı, Turkey)
Board 23	Relationship between soil water potential and sorptivity in a clay soil **Gülay Karahan** and Sabit Ersahin (Cankırı Karatekin University, Cankırı, Turkey)
Board 24	Relationship between spatial resolution and accuracy of predictive maps comparing Soil Survey Geographic (SSURGO) Database aggregation and Terrain Attribute Soil Mapping (TASM) Zamir Libohova (USDA), Laura Bowling, Phillip R. Owens, Hans E. Winzeler (Purdue University), Philip Schoeneberger, **Skye Wills** (USDA)

Board	Title/Author
Board 25	**A model for estimating soil thermal conductivity from texture, water content, and bulk density at moderate temperature** **Yili Lu**, Tusheng Ren (Agricultural University, Beijing China), Sen Lu (Academy of Forestry Sciences, Beijing), Robert Horton (Iowa State University)
Board 26	**Soil and root microbiota of field-grown tomato at various spatial, temporal, and pathological scales** **Nilesh Maharaj**, R.M. Davis (University of California, Davis), E.M. Miyao (University of California Cooperative Extension, Yolo County), J.H.J. Leveau (University of California, Davis)
Board 27	**Improving arsenic phytoremediation efficiency under heterogeneous field conditions: Effects of fertilizer on brake fern arsenic accumulation and biomass production** **Sarick Matzen** (University of California, Berkeley), A. Olson (Santa Fe Right-of-Way Community Partnership), C. Pallud (University of California, Berkeley)
Board 28	**Estimating leaching of water and nitrate below the root-zone of multiple crops using a combination of field instrumentation and modelling** Barzin Ahmad Moradi, Mathew Dumlao, Martin Burger, **Mazier Kandelous**, Wendy Silk, Jan W. Hopmans (University of California, Davis)
Board 29	**Soil organic carbon responses to multi-nutrient addition** **Charlotte E. Riggs** (University of Minnesota, Twin Cities)**,** R.J. Williams (Iowa State University), Nutrient Network (Various Institutions)
Board 30	**Decreasing fertilizer use by optimizing plant-microbe interactions for sustainable supply of nitrogen for bioenergy crops** **Marcus Schicklberger**, Stefan Jenkins, Trent Northen, Dominique Loqué, Romy Chakraborty (LBNL)
Board 31	**Soil Systems for up scaling saturated hydraulic conductivity (Ksat) for hydrological modeling** **Philip Schoeneberger**, Zamir Libohova (USDA), Laura Bowling, Phillip R. Owens (Purdue University) Doug Wysocki, Skye Wills, Candiss Williams (USDA)
Board 32	**Miracle in the vadose zone of onsite wastewater treatment systems: understanding soil processes complexity in remediating wastewater-borne contaminants** **Gurpal S. Toor**, Mriganka De, Sara Mechtensimer, Yun-Ya Yang (Gulf Coast Research and Education Center, University of Florida, Wimauma), P. Chris Wilson (University of Florida, Fort Pierce)
Board 33	**Optimizing monitoring and remediation strategies at the Savannah River Site F-Area, using the Advanced Simulation Capability for Environmental Management (ASCEM)** **Haruko M. Wainwright**, Sergi Molins, Jim Davis, Bhavna Arora, Boris Faybishenko, Susan S. Hubbard (LBNL), Greg Flach, Miles Denham, Carol Eddy-Dilek, David Moulton, Konstantin Lipnikov, Carl Gable, Terry A. Miller, Mark Freshley (LBNL)
Board 34	**Does the concentration of ammonical N fertilizer affect N_2O production in soil? Why?** **Xia Zhu**, Martin Burger, William R. Horwath (University of California, Davis)

Theme 1: Complex Soil Systems – Fundamental Concepts

Mucilage: The Hydraulic Bridge Between Roots and Soil

A. Carminati, M. Zarebanadkouki, E. Kroener, and M.A.A. Ahmed

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As plant roots take up water and the soil dries, water depletion is expected to occur in the soil near the roots, the so-called rhizosphere. Ultimately, as the soil hydraulic conductivity drops and the soil cannot sustain the transpiration demand, roots shrink and lose contact to the soil. Both, water depletion in the rhizosphere and formation of air-filled gaps at the root-soil interface potentially limit the availability of water to plants. How can plants overcome these potential hydraulic barriers at the root-soil interface?

One strategy consists in the exudation of mucilage from the root tips. Mucilage is a polymeric gel that is capable of holding large volumes of water. When exuded into the soil, mucilage remains in the vicinity of roots, thanks to its relatively high viscosity and reduced surface tension. Because mucilage is mainly made of water, its slow penetration into the soil results in higher water content and hydraulic conductivity of the rhizosphere compared to the adjacent bulk soil. Recent measurements with a root-pressure-probe technique demonstrated that mucilage exudation facilitates the water flow in dry soils. Additionally, mucilage increases the adhesion of soil particles to the roots, reducing the formation of gaps at the root-soil interface. Based on these observations, it is very tempting to conclude that mucilage acts as an optimal hydraulic bridge across the root-soil interface.

However, as mucilage dries and ages, it turns hydrophobic. Consequently, the rhizosphere becomes water repellent and its rewetting time increases. Our previous experiments showed that after irrigation subsequent to a drying cycle, the rhizosphere of lupines remained markedly dry for 2 days. Recently, we demonstrated that the rhizosphere water repellency is concomitant with a decrease in local water uptake of 4-8 times. We conclude that after drying and rewetting, the rhizosphere temporarily limits root water uptake.

In summary, the hydraulic properties of the root-soil interface changes over time and along the root system. Young, well-hydrated mucilage optimally connects the roots to the soil and facilitates the uptake of water from relatively dry soils. However, as mucilage ages and dries, it reduces the rhizosphere wettability and the water flow to the roots. This dual behavior of the rhizosphere, rather than a contradiction, seems a plant strategy to adapt to the typically heterogeneous distribution of water in soils. For instance, in a soil profile with water stored in the subsoil, mucilage would facilitate the water uptake of young, deep root segments, and it would avoid water loss from the root segments into the dry top soil.

These studies show that the root-soil interactions in the rhizosphere play a crucial role in regulating root water uptake. We believe that better understanding and management of such interactions can bring to a more efficient and sustainable use of water resources.

A Theory of Soil?

John W. Crawford

Director of the Sustainable Systems Program, Rothamsted Research, UK

We now know that the strength of the interactions between physical, chemical, and biological processes in soil is sufficiently strong to power feedback loops that support complex dynamics in the soil system. Recent work has demonstrated the kinds of behaviour we might anticipate, and this in turn is informing the design of new kinds of critical measurements. The rewards of new insights are profound, and relate to an understanding and optimal augmentation of the natural fertility of soil, including more efficient water and nutrient management, and increased resilience in production systems.

In taking soil science to this new level, it is essential to embrace the complexity that underlies this behaviour, and here we need theory to guide intuition and experimentation. A particularly challenging issue is to decide where the soil system stops and the rest of the ecosystem begins, and what needs to be included in such a theory and what can be left out. In the words of John Muir, the famous naturalist, Scotsman, and founder of the Sierra Club in the U.S., *"When we try to pick out anything by itself, we find it hitched to everything else in the universe."*

Given it is unlikely that we can unhitch soil from the universe, what is the nature of a theory of soil sufficiently general that it can incorporate the rest of the ecosystem (including humans), but sufficiently specific that it can be implemented in practice? In physics, the basis of a dynamical theory is a potential function that completely describes the dynamical state of the system and its resilience. Sustainability and resilience in environmental systems is usually described in terms of optima (i.e., minima) and tipping points respectively on such potential functions, and yet we do not know what the functions or the state variables are. In this presentation, I will explore the concepts of the soil phenotype and critical-zone metabolism as a means of articulating a theory for soil based on flow of nutrition, information, and self-organization. Such a theory might combine ideas from stoichiometry, optimal foraging theory, and the geometric theory of nutrition, with the main outstanding conceptual challenge to link optima at the level of the individual to the structure and function of communities.

Influence of Soil Bacteria on Nitrogen Uptake and Transfer by Arbuscular Mycorrhizal Fungi

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Arbuscular mycorrhizal fungi (AMF) associate with most terrestrial plants and can influence ecosystem ecology and nutrient cycling. There is evidence that AMF can take up soil nitrogen (N) and transfer it to plants. However, many aspects of this process are poorly understood, including the factors that control AMF access to N stored in soil organic matter. This research investigates the influence of bacterial communities on AMF N uptake, and subsequent N delivery to plants. Stable isotope labelling, root exclusion, and spatial analyses are being used to assess the transfer of N from ^{15}N-labeled organic matter to *Brachypodium distachyon* plants that have been inoculated with *Glomus intraradices* and different soil bacterial communities.

A New Worldview of Soils

Henry Lin

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A fundamental shift is needed in our basic thinking and approach towards understanding and managing complex soils to achieve sustainability. After the Newtonian and Darwinian worldviews, a third worldview has emerged that integrates living and nonliving entities as well as space and time cultures. This new worldview emphasizes the interwoven nature of conservation and evolution, the intimate link between internal organization and system function, the systems between extremes, and the unprecedented impacts of anthropogenic activities. Such a new worldview helps the understanding and appreciation of soils as complex, semi-living systems essential to the sustainability of ecosystem services and human livelihood. In the spectrum of things in nature that range from nonliving to living, soils fall right in the middle—functioning as the bridge between the biotic and the abiotic worlds and possessing enormous internal power as the nurturing ground for life. The co-evolution of fast and slow processes in soils is nature's way of sustainable development, where hidden forces drive natural succession, and nonclosed fluxes lead to structural and informational accumulation needed for sustainable functioning. A new kind of physics is needed for enhanced understanding of soil complexity, including (1) the modification of Newton's three laws of motion, (2) the internal organization (rather than externality) of soils in response to perturbations, and (3) the medium number syndrome (systems too complex for classical analytics and too organized for statistical treatment). Soils are a great subject for complexity and sustainability study, where nonclosed cycles and irreversible thermodynamics prevail. However, modern soil vulnerability to global change and anthropogenic threats is unprecedented—if current land-use trends are not adjusted, we may run the risk of losing the ground for sustainability. This paper calls for innovative investigations towards building better human systems that are in harmony with functional natural systems, including soils.

Motility in Water Films and Trophic Interactions Shape Self-Organization of Microbial Consortia on Hydrated Soil Surfaces

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Microbial life in soil occurs within fragmented pore spaces and aquatic habitats where motility is restricted to thin liquid films that may support cell motion for relatively short hydration windows (following large wetting events). The limited ranges of self-dispersion, and the physical confinement, promote spatial association among trophically interdependent microbial species. Considering competition and preferences for different resources and byproduct dependencies of multispecies microbial communities, the spatial organization required for the functioning of such complex diffusion-driven system remains unclear.

We report a mechanistic modeling study of competing multispecies microbial communities grown on hydrated soil surfaces. Model results show how trophic dependencies and cell-level local interactions within patchy diffusion fields lead to niche partitioning that promote spatial self-organization of motile microbial cells. The spontaneously forming patterns of segregated, yet coexisting species, were shown to be robust to spatial heterogeneities and temporal perturbations (hydration dynamics), and responded primarily to the type of trophic dependencies and boundary conditions. The spatially self-organized consortia form ecological templates (patterns) that optimize substrate utilization and could form the basis for more permanent microbial colonies attached to soil surfaces. Limitations to cell displacement ranges and to substrate diffusion give rise to hydration-mediated critical separation distances for the activation of spatial self-organization (i.e., members separated beyond a certain distance do not “join” the consortium).

Preliminary observations to quantify microbial dispersion rates under different hydration conditions, and formation of microbial community patterns on model porous surfaces, will be presented. The study provides new mechanistic insights into how differences in substrate affinities among microbial species could give rise to a remarkable spatial and functional order in an extremely heterogeneous soil microbial world.

Acid Phosphatase Activity in the Rhizosphere: How a Cereal and a Legume Create Local Hotspots

Sarah Placella[1], Gabrielle Daudin[1], Naoise Nunan[2], Esther Guillot[3], Josiane Abadie[3], Camille Gros[1], Claire Marsden[4], and Philippe Hinsinger[1]

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Phosphorus is a poorly mobile, essential nutrient in terrestrial ecosystems. Phosphorus can be of greater local availability in the rhizosphere, where greater biological activity can increase enzymatic activities and induce chemical changes (such as in pH). However, many rhizosphere processes occur at a very fine (millimetric) scale, while sampling is difficult to do at less than a centimeter scale. Using rhizoboxes with 2D access to the soil profile, we mapped acid phosphatase activity *in situ* in chickpea and durum wheat, sole and intercropped, as well as in bare soil rhizoboxes over 5 weeks, from small plants to a post-seed set. We also monitored pH at the very fine (millimetric) scale several times a week, using optodes to understand fluctuations as well as the development of pH shifts in the soil over time and with plant passage. Greater acid phosphatase activity was frequently observed near roots, especially chickpea roots, some root apices, and nodules. We also observed heterogeneity in hotspots of acid phosphatase activity within the soil, and investigated the size and frequency of these hotspots using geostatistics. We combined these results with data on pH to try to understand how rhizosphere processes impact local P availability, and how these processes may shift when different plant species interact with each other.

Peat: A Complex Soil with Dual-Porosity Media

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Soil type is an important factor defining terrestrial ecosystems: it plays a major hydrological, ecological, microbial, and biochemical role with respect to the movement of materials and cycling of carbon, energy, and nutrients. In structured soils, individual aggregates form a network of interconnected microenvironments hosting diverse microbial communities may have different biogeochemical characteristics. Peat soil is an example of structured and highly complex porous (up to ~95%) media, and its physical and hydraulic properties are unique. Peat has complex pore structures that contain a dual-porosity with open, dead-end pores and pores that are closed or partially closed. Pore sizes in undecomposed peat can exceed 5 mm, with sample shrinkage occurring during dewatering. This unique physical property influences the flow and transport characteristics through peat. The advective flux occurs through the hydrologically active fraction of the total porosity (e.g., open and connected pores). However, peat is also capable of attenuating solute flux through diffusion into the closed and dead-end pores comprising the immobile porosity, or through adsorption onto the peat surface. In such complex porous media, nutrient cycling is dependent on interplay between hydrodynamic transport (advection and diffusion) and biogeochemical reactions. Understanding the rate of water flow and solute transport through peat is needed to characterize peat properties and their heterogeneity, for measuring and predicting complex flow processes at the field scale in peatlands. In this presentation, we discuss the effects of peat physical properties and its dual-porosity structure on geochemical, microbial, and biological processes through peat, and also present advanced experimental and modeling techniques to understand the processes in such complex soil systems.

Geochemical and Microbiological Complexity in Soil-Sediment Redox Oscillations

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The input of oxidants relative to utilizable organic carbon controls the predominant terminal electron accepting process(es) [TEAP(s)] in a given soil or sediment horizon. Where the flux of oxidants and organic carbon are relatively constant, sequential organotrophic consumption of electron acceptors (primary redox reactions) leads to the formation of stable redox gradients. However, in hydromorphic soils and hydrologically active subsurface environments, periodic introduction of oxidants into reduced sediments can lead to major alteration in the speciation of redox-active components. The regeneration of oxidized species during redox oscillations (secondary redox reactions) can alter carbon flow pathways during subsequent periods of lower oxidant input. Together, these processes constitute a complex system of feedbacks that can lead to the hot spots of biogeochemical cycling at various spatial and temporal scales in soil and sedimentary environments.

This talk will present the results of numerical experiments conducted with a biogeochemical reaction model that takes into account both primary and secondary redox reactions, as well as the growth and decay of microbial populations involved in organic carbon oxidation. The model is capable of simulating redox oscillations of arbitrary complexity. Preliminary simulations suggest the potential for unexpected temporal feedbacks between oxidant (e.g., oxygen, nitrate) input, microbial biomass growth and decay, and regeneration of oxidized species that can serve as electron acceptors for anaerobic respiration. Application of methods from nonlinear dynamics and chaos to simulation results is under way, with the goal of evaluating the development of phase space structures/attractors and synchronized oscillations of microbial populations in relation to carbon and oxidant concentrations.

Soil Chronosequence Elucidates Development of Soil Structure Heterogeneity

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Quantifying the biogeochemical evolution of soils during pedogenesis is an important step towards the understanding of the mechanistic processes involved in soil development. Soils of marine terraces near Santa Cruz, CA, with soil ages ranging from 60 ka to 225 ka, provide a superb natural laboratory to study soil development (White et al., 2008). These soils developed on relatively homogenous sediments, as still seen in the youngest soil. The oldest soils exhibit prominent reticulate mottling in the B-horizon with striking color segregations, here designated as gray, orange, and white. Mottling is characterized by self-organized heterogeneity on a centimeter-to-decimeter scale. Unlike redoximorphic mottles, which form in carbon-rich oxygen-poor low-lying soils, the carbon-poor Santa Cruz terrace soils are well oxygenated during most of the year—although perched water tables do form during the (Mediterranean climate) rainy season. The goal of this study is to deduce a mechanistic model of mottle formation.

Differences in the physical and chemical characteristics between the various mottle zones, identified by colors, are presumably indicative of the processes through which the self-organizing structures have formed. Separates of mottles by color have measurable differences in particle size, carbon content, Fe isotopes, specific surface area, and mineralogy (by X-ray diffraction). White and orange mottles are silty-sand in grain size, whereas the gray mottles have a high clay content and surface area more than twice that of the other colors. The average Fe concentrations of the mottles are: gray 0.63%, white 1.22%, and orange 4.74%. The average C contents are gray 0.21%, white 0.08%, and orange 0.10%. Higher C content in the gray mottles is suggestive of more root and fungal activity in the gray mottles. The XRD data are consistent with the gray zone being highly weathered with fewer primary minerals. We hypothesize that development of mottling in these soils is the result of long term rhizogenic reactions (after Fimmen et al., 2008). Root and fungal exuded organic acids reduce pH, mobilize Fe and other metals through organo-metal complexation, and begin a cascade of microbial and chemical reactions which (over time) results in morphological heterogeneity.

Fimmen, R. L. et al. (2008). "Rhizogenic Fe-C redox cycling: a hypothetical biogeochemical mechanism that drives crustal weathering in upland soils." Biogeochemistry 87:127-141.

White, A. F. et al. (2008). "Chemical weathering of a marine terrace chronosequence, Santa Cruz, California I: Interpreting rates and controls based on soil concentration-depth profiles." Geochimica et Cosmochemica Acta 72: 36-68.

Soil Microbial Heterogeneity at the Micrometer Scale

N. Taş[1], G. Birarda[1], M. Voltolini[1], S. Wang[1], H.-Y. Holman[1], J. Ajo-Franklin[1], J.K. Jansson[2], and E.L. Brodie[1,3]

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The majority of studies attempting to link soil chemistry and microbial community composition or function are performed using homogenized bulk samples. This approach averages fine-scale (μm) spatial interactions that may be key to understanding patterns of microbial distribution and activation in soils that underlie processes typically observed at much larger (centimeter-meter scales). The aim of this study was to develop approaches to connect μm-scale variations in soil physical, chemical, and biological properties to determine how they may interact to regulate C and N biogeochemical cycles.

To this end, we collected soils from Konza Prairie Biological Station, Kansas. Soil aggregates were manually sorted under sterile conditions into six size classes (100, 200, 300, 400, 500, 1000 μm). The physical structures of six individual microaggregates of 200 μm size were characterized using synchrotron X-ray microtomography (SXR-μCT) at the beamline BL8.3.2. at the Advanced Light Source (ALS). Fourier Transform Infrared (FTIR) spectroscopy equipped with an ATR (Attenuated Total Reflectance) prism was used for high sensitivity chemical imaging and nondestructive classification of 20 (~1 mm) aggregates. Finally, DNA was extracted from individual aggregates of all size classes and further analyzed via 16S rRNA gene iTag sequencing, to determine microbial composition at the aggregate scale. Cluster analysis of FTIR spectra identified two primary clusters of aggregate types based on chemistry (chemotypes) that were distinguished primarily by silicate composition, with hydrated calcium aluminates and silicate hydrates being identified as deterministic spectral features. SXR-μCT imaging revealed highly complex pore networks where the habitable pore space within an aggregate was greater in the interior regions relative to regions near the aggregate exterior. 16S rRNA gene sequencing showed a large variation in phylogenetic diversity between different aggregate size classes. In general, microbial richness or diversity was positively correlated with aggregate size class, demonstrating that, like macroorganisms, soil microbes exhibit positive species area relationships. Specific members of the microbial community showed a strong preference for aggregates of different size, an observation supporting the concept of niche differentiation at the micrometer scale. Ongoing work in this project is focused at determining whether a generalizable set of rules exist to describe microbial distribution at the microbial scale in soils and to use these rules to define new mathematical representations of microbial function in these complex systems.

Panarchy in Soil Systems: Towards Evaluating Resilience Across Multiple Spatial Scales

Morgan M. Williams

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Many soils possess an inherent capacity to recover functional and structural integrity after perturbation. While the resilience of soils is generally appreciated among pedologists, the dynamic and heterogeneous nature of soil systems has made efforts to characterize resilience operationally challenging. Adding to this complexity, soils function at a continuum of spatial and temporal scales regulated by scale-distinct physical, chemical, and biological interactions. In the effort to decrease the negative consequences inflicted upon soil-regulated ecosystem services from increased and variable perturbations due to climate change, additional efforts to understand resilience in soil systems are needed if we wish to decrease climate risk through soil management.

Herein we propose a conceptual framework that can be used to characterize soil resilience at distinct spatial and temporal scales, ranging from the microaggregate (in seconds) to the landscape (in centuries) as organized by a Holling Panarchy of individually nested adaptive systems. Acknowledging the nested, dynamic and adaptive nature of soil systems allows for a more thorough characterization of cross-scale communication and feedbacks, resulting in a more comprehensive understanding of broad system resilience. Such an approach may lend itself to better identifying dynamic thresholds and stable states in soil systems, with implications for targeted management across scales.

Theme 2: Advanced In-Situ Soil Characterization and Experimentation

Probing Microbial Territorial Disputes Using Advanced Correlative Imaging Technologies

Manfred Auer

Life Sciences Division
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One key question for soil microbial ecologists is: What mechanisms do microbes employ to respond when faced with prey, competitors, or predators?

Interspecies bacterial communication and community-wide signaling in response to environmental cues are among the least understood, yet most important, aspects of microbial community life. We currently do not know whether bacterial cells in a biofilm coordinate their metabolism under base conditions, whether they change their metabolism as a response to exposure to other species, and whether local encounters trigger a local or entire community response. We have chosen *Myxococcus xanthus* biofilms as a model system to explore such questions, because *M. xanthus* is not only a ubiquitous soil bacterium, but also one of the best-understood social organisms displaying complex coordinated behaviors, such as social motility and coordinated predation of other bacterial species, as well as fruiting body formation upon starvation. Furthermore, *M. xanthus* is well-known to produce a large arsenal of antimicrobial small-molecule substances, presumably to defend itself.

By integrating small molecule mass-spectrometry and fluorescence-tagged reporter-molecule optical microscopy, as well as fluorescence imaging and electron microscopy, we examined territorial disputes between *M. xanthus* and a variety of other species, including *B. subtilis*.

We found that the ability to form exopolysaccharides (EPS) was crucial to success in territorial disputes, since EPS minus strains are usually outcompeted by the EPS-producing neighbors. Furthermore, we found pair-wise interactions where the bacterial colonies kept a significant distance from one another, whereas in other systems they grew intimately close to one another. When growing close, each colony retained its own territorial identity, with only occasional crossing over of individual bacteria. Interestingly, when the colonies kept their distance, the zone between the bacterial colonies was not completely empty, but rather filled with a dense array of secreted outer membrane vesicles and stacks of lipid membranes, and possibly EPS, creating a very large physical barrier between the two species. When *M. xanthus* encountered *B. subtilis*, we observed the regional secretion of small antimicrobial secondary metabolites in the interaction zone, suggesting that upon contact, *M. xanthus* prepares a chemical response to the external threat, apparently delivered in the form of secreted outer membrane vesicles, as suggested by LC/MS analysis of isolated vesicles.

These results suggest that common soil bacteria utilize a range of mechanisms to erect physical and biochemical barriers, in order to maintain biofilm integrity in territorial disputes.

Mapping potential metabolic interactions among soil bacteria using exometabolomics

Richard Baran[1], Benjamin P. Bowen[1], Megan A. Danielewicz[1], Tami Swenson[1], Stefan Jenkins[1], Romy Chakraborty[1], Ulisses Nunes Da Rocha[1], Eoin L. Brodie[1], Jazmine Mayberry-Lewis[2], Hinsby Cadillo-Quiroz[2], Ferran Garcia-Pichel[2], Adam P. Arkin[1], Adam M. Deutschbauer[1], Trent R. Northen[1]

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Metabolic interactions among soil bacteria are key determinants of global biogeochemical cycles of carbon and nitrogen, however, these interactions are poorly understood. We performed untargeted mass spectrometry based metabolite profiling of cell extracts and spent media of key soil bacterial isolates to characterize metabolites produced or released by these strains. Afterwards, selected individual isolates were cultured in complex media and metabolite profiles of spent media were compared to metabolite profiles of control media to detect utilization or release of metabolites. Metabolite extracts of studied isolates or metabolite extracts of authentic soil were used as supplements in complex media to include previously uncharacterized metabolites which may be relevant under environmental conditions. We identified a set of metabolites utilized by essentially all studied isolates showing a potential competition for these compounds in the soil. Individual isolates utilized only subsets of compounds from complex cell or soil extracts showing a specialization towards specific metabolites. This broad scope molecular level study of potential metabolic interactions within microbial communities may improve the understanding of the dynamics organic matter in the soil.

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Mass Spectrometry Approaches for Analysis of Soil Organic Matter Composition and Bacterial Cycling

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Microbial mineralization of soil organic matter (SOM) is a key determinant of global biogeochemical cycles of carbon and nitrogen. However, the chemical composition of SOM and the mineralization of its components by specific soil bacteria are poorly understood. Mass-spectrometry-based metabolomic methods have the potential to resolve these chemical components and enzyme activities to improve our understanding of carbon cycling in soils. Here, we describe mass-spectrometry approaches for the untargeted metabolite profiling of soil metabolites, and examination of the activities of key isolate bacteria against soil metabolites. This was accomplished by culturing soil isolates in complex media. Then we compared exometabolite profiles of spent media to metabolite profiles of control media to detect uptake or release of metabolites. Metabolite extracts of studied isolates or metabolite extracts of authentic soil were used as supplements in complex media, to include previously uncharacterized metabolites that may be relevant under environmental conditions.

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Moving Away from the Geostatistical Lamppost: Why, Where, and How Does the Spatial Heterogeneity of Soils Matter?

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Since the late 1970s, thousands of scholarly articles, books, and reports have applied the mathematical theory of geostatistics to characterize the spatial "variability" of soils, and to produce soil-property maps. Insensibly, this application of geostatistics appears to have become an end in itself—the reasons why one should be concerned about the spatial heterogeneity of soil properties are rarely if ever made clear anymore. In this context, the purpose of the present talk is to return to some of the primal questions that motivated this interest in the topic several decades ago.

After a brief review of the background behind the application of geostatistics to soils, we describe a number of situations and modeling efforts in which, even though soils undoubtedly vary spatially, nothing seems to be gained practically by explicitly accounting for their spatial heterogeneity, in order to reach a number of management or research objectives. In contrast, whenever the spatial heterogeneity of soil properties in a field might be relevant, it is shown that very different perceptions about it emerge, depending on the type of measurement that is performed. This suggests that the approach one adopts to characterize spatially varying soil properties should be dictated by whatever goal one is pursuing. For example, if the objective is to evaluate the "ecosystem services" of soils in a given region and to reach decisions about them, one should probably first consider the (typically large) spatial scale that is most relevant to the decision-making process, then proceed via a top-down approach to characterize the spatial heterogeneity of soil services, if and when appropriate. In other contexts, it is argued that measurements should be patterned after the behavior of plants or microbes present in soils, relative to which, unfortunately, the macroscopic measurements that are now routinely carried out appear largely irrelevant or misleading. The talk concludes with a number of potential lessons learned from our analysis of the research on the spatial heterogeneity of soils, which bear relevance to the broader practice of soil science.

Assessment of Soil Bacterial Diversity Patterns in the Mediterranean Ecosystems of Crete (Eastern Mediterranean Basin)

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The Mediterranean Basin is considered among the “hot spots” for plant biodiversity worldwide: 10% of the world’s higher plant species can be found in an area representing only 1.6% of the Earth’s land surface. Furthermore, endemism also reaches high levels in the Mediterranean Basin: ~52% of the vascular plant species there are found nowhere else in the world. Considering the coexistence and close interactions of plant and microbial communities, it is of interest to investigate whether microbial communities also have high levels of diversity in Mediterranean ecosystems, whether such microbial communities follow vegetation patterns, and how microbes are involved in Mediterranean ecosystem functions. Difficulties in the study of microbial diversity and functions in the terrestrial ecosystems of the Mediterranean Basin mainly arise from the fact that the environmental heterogeneity and complexity of these ecosystems is very high, the methods used have various inherent biases, and the distribution of Mediterranean ecosystems in many countries, requiring coordination and common research efforts. The aims of this study were to gain insight into the spatial patterns of bacterial genetic diversity in Mediterranean ecosystems on Crete, and to correlate these with data on climate, vegetation, and nutrient states. Our experimental design was based on the main habitat types found in Crete, classified according to the habitat type classification scheme of NATURA 2000 and including the following: *Sarcopoterium spinosum phrygana*, *Oleo-Ceratonion* forests, *Acero-Cupression* forests, Oromediterranean phrygana with heaths and gorse, Greek briar woods (Dehesas), and Mediterranean Pine forests. Soil samples were collected from 11 sites. To assess and evaluate soil bacterial genetic diversity, we based our experimental approach on T-RFLP (Terminal Restriction Fragment Polymorphism), Cloniung/Seqencing techniques and PhyloChip (phylogenetic microarray), using the 16S rRNA gene as a molecular marker. Additionally, we evaluated and compared the discriminating power of the molecular techniques used. The spatial differentiation of genetic diversity, along with the relationships among other factors, provides insights into the possible role of bacterial communities in the Mediterranean ecosystems of Crete.

Tracking the Temporal Dynamics of Cellulose Utilization by Bacteria and Fungi in Soil Using ^{13}C-stable Isotope Probing and Next-Generation Sequencing

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We have limited knowledge of the contributions of specific microbial taxa to carbon (C) cycling in soil systems, which traditionally has depended on the need for microbial enrichment and isolation. Nucleic acid stable isotope probing (SIP) facilitates the tracking of carbon flow through microbial communities. We employed an approach in which a complex C mixture simulating soil organic matter was added to soil microcosms. Constituents of the added C mixture were systematically replaced with their ^{13}C-labeled equivalents, enabling the elucidation of C use patterns by specific microorganisms. In this experiment, we focus specifically on microbial metabolism of ^{13}C-labeled cellulose in soil. Using CsCl isopycnic density gradient centrifugation and fractionation, we measured incorporation of ^{13}C into microbial DNA over a period of 30 days. Bacterial small subunit rRNA gene sequences and fungal internal transcribed spacer (ITS1) region sequences from 20 CsCl gradient fractions for each treatment and time were characterized by next-generation sequencing and classified into Operational Taxonomic Units (OTU). OTUs that assimilated cellulose were identified using ordination analyses, and patterns of isotope incorporation were measured over time for each OTU. Bacterial incorporation of ^{13}C from cellulose was observed after 14 days with highly responsive phyla including *Proteobacteria* (including the canonical cellulose degrader *Cellvibrio*), *Chloroflexi*, and *Verrucomicrobia*. However, substantial respiration of cellulose was observed prior to Day 14 with loss of 13% of cellulose ^{13}C by Day 3, 21% loss by Day 7 and 48% by Day 14, indicating cellulose utilization well before incorporation of ^{13}C into bacterial DNA. To determine whether fungi were responsible for cellulose degradation at early time points, we assessed the incorporation of ^{13}C into the DNA of fungal taxa by next-generation sequencing of fungal ITS1 regions from gradient fractions used for analysis of bacterial DNA. These results reveal the temporal dynamics of cellulose degradation by bacteria and fungi in soil over time.

Experimental Studies of Ambient-level Noble Gas Dynamics in Porous Media: Fractionation and Evaluation of Transport Mechanisms through Advective-Diffusive and Dusty Gas Models

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In order to evaluate fractionation of vadose zone “stagnant” gases in the presence of an advective-diffusive flux, a dry sand-filled column experiment has been devised where pure CO_2 can be injected at the base of the column and maintained at constant flow rate. The experimental apparatus allows for variable CO_2 fluxes through a column in which ambient pressures can be measured and gas samples collected at pre-determined depths. Prior to initiation of CO_2 flux, the ambient “stagnant” gases throughout the sand column are equilibrated with the atmosphere, which also establishes the sand-surface boundary condition. The gas samples collected during the flux experiment are analyzed for noble gas concentrations. These values are compared against their atmospheric abundances, providing a measure of the fractionation factors for each of the five stable noble gases as a function of depth and CO_2 concentration and flux. We evaluate the internal relationship among “stagnant gases” during transport through a porous media and the factors that control noble gas fractionation in terms of both an advective-diffusion and a dusty-gas model.

A preliminary result obtained under high flux conditions (10,135 gm m^{-2} day^{-1}), found that the degree of noble gas fractionation was consistent with values predicted from the dusty gas model. We are now in the process of gathering more detailed data as a function of sampling depth and flux. By varying the CO_2 flux, we can observe how noble gas responds to a shift from diffusive to advective dominated transport. This study also enables evaluation of computed fluxes based on Fick’s law (ordinary diffusive flux), Darcy’s law (ordinary viscous flux), and knudsen flux, and shows the variation in flux components as a result of CO_2 flux changes, which indicate how the coupled nature of viscous and diffusive mechanisms control CO_2 and noble gas concentrations and transport though porous media.

Complexity in Soil Biogeochemical Processes Arising from Aggregate-Scale Heterogeneity

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Soils are one of the most complex materials on Earth. On a volume basis, they harbor the greatest biological diversity on the planet that exists within an intricate mineralogical/chemical system and convoluted physical framework—all of which combine to make soils and soil processes complex. Processes controlling elemental cycling within soils are thus governed by a combination of chemical and biological factors, as constrained by physical aspects of the system. We recognize that soils differ greatly on a geographic basis and indeed within an individual profile on a horizon basis. Less obvious (typically) is the heterogeneity arising at the aggregate level, what may be argued as the fundamental unit of heterogeneity operating within soils. Here, chemical gradients arising from physical structure are at their greatest, leading to large differentials in biological processes and metabolisms. Along aggregate exteriors, macropores supply nutrients and oxygen (via aeration) to the greatest extent, but also are subject to the most rapid decrease in moisture levels. Moving toward aggregate interiors, a progressive decrease in aeration is found and, for subsurface horizons where aggregate turnover is slow, a decrease in nutrient and organic carbon supply. The impact of aggregate-scale heterogeneity in soil processes is well illustrated by comparing the seemingly simplistic microbial reduction of the iron oxide ferrihydrite within an aggregate with an advective flow system. Under a homogenous advective flow regime, ferrihydrite transforms uniformly to goethite or magnetite, depending on the Fe(II) concentration. By contrast, ferrihydrite transformation within aggregates leads to a spatial distribution of various iron oxides, inclusive of transformation products and remnant ferrihydrite, owing to Fe(II) gradients—a consequence of nutrient and oxygen supply. At the field-scale, aggregate-scale variation in soil processes is most demonstrative in hydric soils, as noted by the classic redoximorphic iron mottles, but they are operational in nearly every soil environment. Using a highly weathered soil where critical nutrient supply occurs along macropores in both surface and subsurface horizons, we illustrate a uniform oxygen level but rapid decrease in microbial activity within aggregate interiors. By contrast, within aggregates of surface and subsurface horizons of a Mollisol, oxygen rather than nutrient supply limits (or alters) microbial activity, and in this case specific redox metabolisms. In sum, whether nutrient rich or poor, the physical structure of soils leads to vast changes in microbial metabolism and chemical conditions. Thus, in order to capture the complexity of soil processes, we have to scale from the aggregate level.

Microbial Community Dynamics in Salt Crusts of the Hyperarid Atacama Desert

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In the hyperarid Atacama Desert, 10 years or more may pass between measurable precipitation events. This extreme environment has produced a landscape devoid of macroscopic life (McKay et al. 2003). For decades, researchers have probed the soils for an indication of life, but to no avail (Navarro-Gonzalez 2003). It soon became known as the dry limit to life, too hostile to sustain any growth (Warren-Rhodes et al. 2006). However, microbial life has recently been discovered there, colonizing translucent halite salt (NaCl) crusts on the surface of evaporitic basins (Wierzchos et al. 2006). Existing work suggests that the presence of halite is key to microbial survival (Wierzchos et al. 2012). This belief relies on a process known as deliquescence, which occurs when ambient relative humidity reaches 75%. Under these conditions, halite is able to absorb moisture from the atmosphere to create a saturated liquid solution (Mauer and Taylor 2010). Coastal marine fog occurs on a regular basis along the Atacama Desert and has been shown to raise relative humidity enough to initiate deliquescence in the crusts (Davila et al. 2008).

Though this fascinating ecosystem has been identified, very little work has been performed to profile the microbial communities. For this study, halite samples were collected from three sites along a fog gradient to examine how community dynamics might change relative to water availability. Total genomic DNA was extracted and bacterial and archaeal taxa identified by analysis of 16S rRNA amplicons using high-density DNA microarrays (G3 PhyloChip™). At the site closest to the coast, which receives the most frequent and intense fog, the greatest relative richness of both bacteria and archaea was observed. The samples from this site also showed the greatest within-site variability. The relative abundances of *Halorubrum* and *Halomicrobium* were variable among the sites. These results suggest there is a positive correlation between water availability and species richness.

Autonomous Millimeter-Scale RFID Sensors for High Density *In-Situ* Soil Monitoring

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Better understanding of plant and microbial communities would be dramatically enabled by an ability to monitor their behavior in-situ, dynamically and in a variety of environments. To address this need, we are designing a mm-scale autonomous sensor platform that can incorporate on-chip and post-processed sensors to be deployed in order to monitor complex soil systems. The sensors are powered using RF energy harvesting with an on-chip antenna and therefore, do not require a bulky battery that needs to be replaced. Recent advances in sensor technologies, which allow a variety of sensor types to be post-processed on conventional CMOS, will expand the quantities which can be monitored. The small size of these sensors allows for high-density monitoring of soil. With in-situ sensing, we hope to enable monitoring of root architecture and growth; root exudates and enzymes; the dynamics of C, N, other nutrients and redox sensitive species; and gas and moisture fluxes among other applications.

Bulk Carbon K-edge X-ray Absorption Spectroscopy: Overcoming Technical Challenges

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Organic matter in soils controls the storage and availability of nutrients and pollutants, water-holding capacity, stabilizes structure and improves tilth, buffers the soil against rapid changes, provides surface protection, and stores carbon. The quality and quantity of soil organic matter (SOM) varies considerably between soils, depending on the type of the original plant material and its transformation through interactions with the mineral and biological components of soils, landscape position, and climate. Characterization of the organic matter is thus essential to effectively manage the soil resource.

X-ray absorption spectroscopy (XAS) at the C K-edge probes the local bonding environment of C, providing information on the types (e.g., aromatic C=C, carboxylic) and quantity of the C functional groups present. While scanning X-ray transmission microscopy (STXM) is being used to quantify and identify the C functional groups in SOM, it is limited, by low throughput, to very thin particles (clays) and low sampling density. Bulk XAS techniques permit for high throughput, the study of whole soils, and high sampling density. In many projects, these bulk XAS measurements may be more pertinent to understanding large-scale processes in soils such as the global C cycle.

However, technical challenges have prevented widespread use of bulk C K-edge XAS for studying SOM. Normalization of the C data is problematic due to carbon contamination of the beamline optics, including the in-line Au mesh initially used for Io. Higher order light in the incident beam, particularly at the O K-edge, contributes to the detected signal. Also, radiation damage due to the high dose rates changes the type and quantity of the C functional groups present in a sample. Hence, deriving quantitative information from the C spectra is limited.

These technical challenges have been largely overcome through the use of energy-selective silicon drift detectors, which enable the carbon signal to be detected separately from the signals from higher order light such as oxygen (i.e., partial fluorescence yield). Accurate normalization is now possible using the X-ray scattering signal from Au-coated Si wafers as the Io, negating the carbon beamline contamination issues. The radiation dose was minimized using rapid scanning in conjunction with the sampling of many spots on a sample. In summary, bulk C XAS is now positioned to contribute significantly to advancing the characterization of organic matter in soils and environmental soil-like samples (e.g., sediments).

Biological Stability of Soil Organic Matter Is Related to Thermal and Chemical Properties

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Soil organic matter (SOM) is a key property that underpins ecosystem productivity, and understanding its physical, chemical and biological properties is important for evaluating its role in carbon (C) cycling in terrestrial ecosystems. The stability of SOM as it relates to resistance to microbial degradation has important implications in ecosystem processes related to nutrient cycling, emission of greenhouse gases from soil, and C sequestration. Thus, there is interest in developing new ways to measure and quantify the labile and stable forms of soil organic carbon.

In this presentation, we describe the combined use of thermal decomposition methods based on pyrolysis, and chemical properties using X-ray absorption spectroscopy (XAS), to describe the stability of SOM. In thermal analysis, the sample is subjected to a temperature ramp, and changes in volatilized organic C are recorded as a function of temperature. Analysis by XAS provides information on the types of C functional groups present in a soil sample. Soils were obtained from sites over a wide geographical range and range of management practices. Controlled respiration studies were conducted on the soils to determine the biodegradability of organic C. We show that biological stability is well described using a two-component model that includes thermal stability and C composition chemistry.

Geophysical Identification and Characterization of Permafrost Soil Functional Zones

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Characterized by a vast amount of carbon stored in the permafrost, warming temperatures, and a rapidly evolving landscape, the Arctic has emerged as an important focal point for the study of climate change. Although recognized as an ecosystem highly vulnerable to climate change, mechanisms that govern feedbacks between the microbially driven terrestrial processes and climate system in the Arctic region are not well understood. Characterization of controlling biological, geochemical, and physical processes that govern the ecosystem functioning is extremely challenging, due to the variable length and time scales involved.

This presentation will discuss a new approach for identifying and characterizing Arctic tundra functional zones over length scales of centimeters to kilometers. The study was conducted as part of the Next Generation Ecosystem Experiment project, which is being carried out in the ice-wedge dominated Barrow Environmental Observatory (Barrow, AK). The approach utilizes above- and belowground geophysical datasets (LiDAR, electrical, GPR, electromagnetic) to characterize properties that are expected to be critical for governing soil microbial respiration (such as microtopography, soil moisture, vegetation density, and active layer thickness). Unsupervised cluster analysis is performed to quantify the co-variability of above- and belowground geophysical responses and to identify regions in the landscape that have unique distributions of important properties. Once these functional zones are identified, we use statistical techniques to explore if particular geomorphic aspects of the functional zones can best explain the variability in observed properties and CO_2 and CH_4 fluxes.

Our results demonstrate the significant microtopography-driven correspondence between the variability of land-surface and subsurface properties in the Arctic tundra. Results show that functional zones can be used to explain spatially variable distributions of carbon fluxes and related properties. The study suggests the value of co-utilization of above- and belowground geophysical datasets for tractably characterizing multiscale zonation over large Arctic ecosystems, and for assessing the variability of the key components in the system. Improving our ability to characterize multiscale Arctic systems is a prerequisite for improved predictions of microbially driven ecosystem feedbacks to the climate.

Sequential Selective Dissolution to Quantify Storage and Stability of Organic Carbon Associated with Different Mineral Types

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Stabilization of SOM (soil organic matter) is regulated in part by sorption and desorption reactions happening at mineral surfaces, as well as precipitation and dissolution of metal-humus complexes. Fe and Al hydroxides play a particularly significant role in SOM stabilization in soils, because of their ubiquitous distribution and their highly reactive surface properties. Fe and Al hydroxides exist in soils across a wide spectrum of crystallinity, ranging from dissolved Fe and Al cations that combine with organics to form metal-humus precipitates, to the more crystalline end members, goethite and gibbsite, which sorb SOM through a variety of molecular interactions. Though the importance of these sorption and precipitation reactions has long been recognized, the distribution of SOM among Fe and Al hydroxides of differing crystallinity has not been well quantified, nor have the time scales over which these stabilization mechanisms operate. In an attempt to measure the distribution of organic C among (i) Al- and Fe-humus complexes, (ii) short-range-order Al and Fe hydroxide surfaces, and (iii) crystalline Fe oxyhydroxide surfaces, we applied a suite of selective dissolutions to soils of four different geneses (a tropical forest Andisol, a temperate forest basaltic Mollisol, a mediterranean coastal prairie Mollisol, and a northern mixed hardwood forest Spodosol). The traditional reactants used in selective dissolutions were replaced with carbon-free analogues, so that the carbon released along with the Fe and Al at each stage of the selective dissolution process could be examined. Selective dissolutions were performed sequentially: Na-pyrophosphate (Al- and Fe-humus complexes) followed by hydroxylamine (short-range-order Al and Fe hydroxides), followed by dithionite/HCl (crystalline Fe hydroxides). C, Al, and Fe concentrations, as well as $\Delta^{14}C$ were measured for the solutions yielded by each stage of the selective dissolution process. $\Delta^{14}C$ data were used to estimate a MRT (mean residence time) for SOM associated with each selective dissolution stage. Results suggest that precipitation of metal-humus complexes (pyrophosphate extractable C) accounts for the largest pool of stabilized C among the three fractions examined (20-95% of bulk soil C), but these complexes had a much shorter MRT than C stabilized through association with SRO and crystalline hydroxides. Sorption to short-range-order and crystalline phases accounted for a small fraction of mineral-stabilized C in temperate soils, in strong contrast to the tropical Andisol, where C associated with short-range-order phases accounted for nearly 25% of bulk soil C. Data suggest that sorption confers a higher degree of stabilization than metal-humus complex formation, though metal-humus complexes account for a larger proportion of the bulk soil organic C pool.

Unearthing Complex Soil Microbial Communities Using Omics

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Soil represents one of the most complex ecosystems on Earth, with a high microbial diversity and structural heterogeneity. Therefore, it has been challenging to study the functional roles of microbial populations within the soil habitat. Recently, the application of omics technologies have been used to explore soil microbial communities and have begun to reveal hitherto unknown soil microbial populations and to link them to specific soil biogeochemical processes. Examples of research areas include study of the impact of altered rainfall patterns on soils of the Great Prairie of the United States, and study of the impact of climate warming on Arctic soil microbial communities. For these projects, we employed an omics pipeline that includes metagenomics, metatranscriptomics, and metaproteomics to determine the phylogenetic and functional gene compositions and their expression in complex, nonsterile soil samples collected from the field. These studies have presented several challenges due to the unprecedented large size of the datasets and the insufficiency of available bioinformatic tools and databases to analyze, correlate, and integrate the data. To address these challenges we developed a novel functional gene database and used different assembly and analysis algorithms to determine key features in the datasets. The data reveal the microbial diversity, composition, and functional potential in the different soil systems, and how the microbial communities respond to climate change impacts.

Meta- and Isolate Genomics for Characterization of Grassland Soil Microbial Communities

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As part of a large effort whose overarching goal is to determine the impact of the interactions between plant roots and soil microbial communities on organic C decomposition and stabilization processes in soil, we are using isolate genomics-assisted metagenomics to define microbial members of soil from a Mediterranean grassland. Soil samples were collected from a Northern California annual grassland after the summer dry season and at the peak of the wet season. Ultradeep shotgun sequencing of samples from each season was performed, yielding a total of nearly 1.5Tb of sequence in ~10 billion Illumina short reads. From the same soils, we recently built a repository of 290 bacterial isolates obtained from multiple dilute media formulations incubated over a period of 2.5 months. Thirty-seven isolates have been sequenced to date, and their draft assemblies have been completed. The severe complexity of soil microbial communities and the required large volume of sequencing data make *de novo* assembly of soil metagenomes very challenging. Here, we report a tiered co-assembly approach leveraging the 37 sequenced isolates. We first mapped shotgun reads from both samples to the isolate genomes and used the mapped reads to generate *de novo* assemblies of the corresponding “wild” relatives. For the remaining unmapped reads, we built an iterative and scalable assembly pipeline using a ray meta-assembler that targets different coverage bins at each iteration. The scaffolds generated from these two approaches are pooled together for downstream differential coverage and k-mer profile-based taxonomic binning (assignment of scaffolds to organisms) as well as metabolic trait extraction.

Monte-Carlo Simulation of Soil Carbon Measurements by Inelastic Neutron Scattering

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Measuring soil carbon is critical for assessing the potential impact of different land-management practices on carbon sequestration. The inelastic neutron scattering (INS) of fast neutrons (with energy around 14 MeV) on carbon-12 nuclei produces gamma rays with energy of 4.43 MeV; this gamma flux can be directly used for determining soil carbon. INS has several advantages over current well-known methods of carbon determination (i.e., dry combustion, laser induced breakdown spectroscopy, mid and near infrared reflectance spectroscopy). The method is nondestructive, no sample preparation is required, and a large soil volume is analyzed in a single measurement. While the theory and methodology of INS has been developed (Wielopolski et al., Brookhaven National Laboratory, 2000-2012), the development and testing of experimental equipment for directly measuring field soil carbon is currently being done at the USDA-ARS National Soil Dynamics Laboratory in Auburn, AL. To increase the accuracy and reliability of this method, a Monte-Carlo simulation of neutron transport and interaction with soil nuclei can be used. The Geant-4 tool kit (S. Agostinelli et al. 2003) makes it possible to develop software for conducting such simulations. In this work, we combined the Geant4-based simulation software for neutron transport and interaction with soil nuclei, with the acquisition of gamma rays by a system similar (i.e., neutron energy, geometry size, detector type and size) to the National Soil Dynamics Laboratory INS system. Using this software, neutron-induced gamma spectra were simulated for soil samples of different sizes, with differing amounts of carbon, and with different amounts of other soil components. Simulation results demonstrated good agreement with experimental data in the dependence of the carbon 4.43 MeV peak areas to the carbon content in soil samples, regardless of sample thickness or the silicon weight percentage of the soil. This agreement verifies the usefulness of this simulation method and offers the possibility of utilizing this method for the analysis of other factors influencing soil carbon measurement by the INS method. For example, the effects of soil moisture, density, and carbon distribution with depth were simulated; the results of these simulations will be discussed.

Synchrotron-Based Characterization at the APS to Determine Physical and Chemical Characteristics of Carbon in the Subsurface and Root Zones to Improve Earth System Modeling of the Biogeochemical Cycling of Carbon

ANL SBR SFA (Laboratory Research Manager: Robin Graham)

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Mechanistic understanding of carbon (C) biogeochemical cycling is essential for the development of Earth System Models. Critical for that mechanistic understanding is determination of physical characteristics and chemical speciation of C in subsurface and root-zone environments. Hard x-ray microtomographic imaging of soil pore structure in soil aggregates is a powerful approach to understanding physical structure and controls of C partitioning within soils. X-ray spectroscopy- and microscopy-based investigations of constituents of subsurface and root-zone materials can provide critical insights into the chemical nature of C in these materials. Although soft x-ray scanning transmission x-ray microscopy (STXM) can provide spatially resolved chemical information about C in samples, the thickness and hydration states of environmental samples often preclude the utility of soft x-rays. This limitation can be overcome with the x-ray Raman technique (separate poster), which enables measurement of C 1s x-ray absorption (XAS) spectra using high energy x-rays. We are integrating x-ray microtomographic, Raman, and STXM approaches to develop a mechanistic understanding of C cycling.

We are investigating the feasibility of locating a soft x-ray STXM beam line as a "side branch" on an APS bending magnet beam line already developed for XAS. Use of x-ray optic components recycled from decommissioned beam lines will drastically reduce the cost of developing such a capability. Integrating these approaches into our research will provide spatial resolution information that will be complementary to x-ray Raman measurements of bulk samples.

We have also investigated the pore space and physical structure of three size classes of soil aggregates (250-425, 425-841, and 841-100 µm) collected from a grassland field to determine correlations between aggregate size, internal pore structure, and microbial community composition within aggregates. X-ray transmission microtomographic measurements indicated a greater proportion of the pore space in the small- and medium-sized macroagregates is present as relatively smaller pores, resulting in greater overall porosity and pore-mineral interface area. Building on this approach, we have also begun technique development with the ultimate goal of imaging the spatial arrangement of microorganisms and metabolic processes within opaque media, such as soil aggregates (separate poster).

Current Understanding and Future Directions: The Form and Function of the Organo-Mineral Interface

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We will review old and new concepts of the organo-mineral interface. Traditional conceptualization of the interface suggests that soil minerals are available for interaction with solutes, except where those minerals are blocked by organic carbon. Surface complexation modeling approaches, common in soil and aquifer reaction networks, generally and explicitly use mineral substrates to represent sorption. Both Langmuir and Freundlich equations represent adsorptive interactions with soils, but both assume monolayer sorption. However, density separations have identified different thicknesses of organic materials on soil minerals, which tend to decrease as a function of increasing density and increase in age and chemical lability. We suspect that the interface consists of a complex architecture of layered, simple compounds. However, direct experimental observations of the interface are lacking. We initiated a set of experiments involving the creation of simple soil mineral-organic analogues, using neutron reflectometry to penetrate layers and identify differences in density as a function of depth, at the nanoscale. We observed the formation of distinct layers of organics in a variety of systems, and found that layer formation is associated with a contrast in hydrophobicity in the compounds and is not sensitive to the order of addition. However, compounds with similar hydrophobicity did not form distinct layers; rather, a mixed layer was formed. We also used molecular dynamics simulation to predict interactions between individual atoms in the system, and found results that were consistent with layer formation observed in the neutron experiments. Our experiments constitute a first step in using a variety of techniques to understand the principles governing the shape and indeed the function of the organo-mineral interface. Considerable work remains, with particular relevance to contaminant and nutrient interactions in aquifers and soils, and the stabilization of organic carbon with respect to microbial decomposition and sensitivity to land use and climate change.

Carbon Chemistry in Unaltered Soil Samples Using Nonresonant Inelastic X-ray Scattering

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Advancing mechanistic understanding of carbon biogeochemical cycling is crucial for predicting future climate change. Characterizing chemical speciation of carbon in unaltered soil samples is critical for assessing the dynamics of carbon cycling in the earth system. Although carbon k-edge x-ray spectro(micro)scopy can provide spatially resolved chemical information about carbon in soil, the thickness and hydration state of environmental samples often precludes the utility of soft x-rays in these studies. Non-resonant inelastic x-ray scattering (NIXS) with a lower energy resolution inelastic scattering (LERIX) instrument enables measurement of carbon 1s x-ray absorption spectra with higher energy x-rays, thus enabling the measurement of thick and hydrated samples without the need for sample containment in a vacuum. We have made NIXS measurements of a variety of carbon-containing material standards, soil constituents, and soil samples. Results indicate that measurements can distinguish important C moieties like aromatic-C, amide-C, phenol-C, carbonyl-C, and carboxyl-C. Results obtained from NIXS are complementary to NMR. Details of these results will be presented.

Belowground Linkages During Ecosystem Development: Patterns of Microbial Community and Organic Matter Change Associated with Pedogenesis

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Ecosystems are complex interconnected systems described by diverse living and nonliving interactions. The development of ecosystems occurs over multiple time scales that include progressive and retrogressive stages. We studied ecosystem development to describe the relationship between microbial communities, vegetation, soil organic matter change, and shifts in amide-N associated with pedogenesis. This study was initiated along a developmental sand-dune soil chronosequence bordering northern Lake Michigan near Wilderness Park (WP) with the hypothesis that microbial communities, vegetation, and shifts in organic matter would show display patterns of change indicative of interconnected ecosystem feedbacks associated with ecosystem development. Five replicate samples were taken from nine soils ranging in age from ~105 to 4010 years since deposition. Whole-mineral soil and mineral-associated heavy fractions (meta-tungstate) were acid-hydrolyzed (6N HCl at 110°C for 24h), purified using SPE and derivatized with a 6-aminoquinolyl-N-hydroxysuccinimidyl carbamate fluorescent tag. Amino acids were analyzed using a high-performance liquid chromatograph equipped with a fluorescence detector. The microbial composition and diversity in the soil was studied using bacterial and fungal tag-encoded FLX amplicon pyrosequencing of rRNA genes. As hypothesized, Bray-Curtis ordination indicated that community assembly and soil-proteinaceous amino acids showed patterns of change related to pedogenesis and vegetative change. Amino acids, the dominant pool (50-80%) of acid hydrolysable organic matter, shifted in association with plant and microbial community dynamics, with basic amino acids (arginine, lysine, histidine), which are polar and positively charged under acidic conditions, showing a clear pattern of accumulation during 4000 years of ecosystem development. Histidine, for example, increased from 1.2% to 2.6% of total amino acids. In contrast, glycine, aspartic acid, and alanine in soil declined from ~17 to 7% with ecosystem development. These results support the concept of interactive feedbacks driving ecosystems. Mineral weathering and the development of acidity, driven by rain and vegetation, support the accumulation of negatively charged soil exchange sites during early progressive and mid-stages of soil development. It is notable that the DNA of plants, fungi, and acidobacteria are relatively enriched in codons for histidine and arginine compared to other bacteria. The increased abundance of these organisms may thus also reflect the shifts in mineral-soil-derived amino acids during pedogenesis. Microbial communities may be the major source of amino acids, but the current working hypothesis is that accumulation of metabolically expensive basic amino acids is mainly a function of preferential chemical binding and enhanced production by microbes.

A Novel Nanoparticle Approach for Imaging Soil Bacteria

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The metabolic activities of soil microbes are the primary drivers of biogeochemical processes controlling the terrestrial carbon cycle, nutrient availability to plants, contaminant remediation, water quality, and other ecosystem services. However, we have a limited understanding of microbial metabolic processes, such as nutrient uptake rates, substrate preferences, or how microbes and microbial metabolism are distributed throughout the three-dimensional complex of the soil. Here, we use a novel imaging technique with quantum dots (QDs, engineered semiconductor nanoparticles that produce size or composition-dependent fluorescence) to measure bacterial uptake of substrates of varying complexity. Cultures of two organisms differing in cell wall structure—*Bacillus subtilis* (a member of the Firmicutes) and *Pseudomonas fluorescens* (a member of the Proteobacteria)—were grown in biofilms in one of four ecologically relevant experimental conditions: nitrogen limitation, phosphorus limitation, nitrogen and phosphorus limitation, or no nutrient limitation. The biofilms were then exposed to QDs with and without organic nutrients attached.

We found that uptake of QDs conjugated to organic substrates varied, depending on growth conditions and substrate, suggesting that they are a useful indicator of bacterial ecology. Cellular uptake was similar for the two bacterial species (2222 ± 273 nanoparticles per cm^3 of cell volume for *B. subtilis* and 1826 ± 278for *P. fluorescens*). Uptake of QDs not conjugated to an organic molecule was negligible, indicating that bacteria actively consume the QD-labeled nutrient rather than QDs passively entering cells. On average, QD assimilation was six times greater when nitrogen or phosphorus was limiting (i.e., the substrate conjugated to the QD-provided nitrogen and/or phosphorus that was experimentally limited in the growth medium). Overall, cells took up about twice as much phosphoserine compared to other substrates, likely because it was the only compound providing both nitrogen and phosphorus. These results showed that regardless of their cell wall structure, bacteria can selectively take up quantifiable levels of QDs based on substrate and environmental conditions. These findings offer a new way to experimentally investigate basic bacterial ecology, such as metabolic activity and biofilm development and function.

LBNL Radiotracer and Imaging Technologies for Microbial Systems Research

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Radiotracers have long been used in environmental sciences to trace specific chemical processes, but now recent use of nuclear medical imaging tools (i.e., gamma camera, single photon emission computed tomography [SPECT], or positron emission tomography [PET]) is expanding the scope of what can be done with radiolabelled compounds, due to the ability to dynamically measure the 3D distribution of radiotracers inside sediment systems, with better than 1 cm resolution and picomolar sensitivity. In this work, we use PET and SPECT to probe acetate metabolism, associated iron reduction, and subsequent technetium reduction in sediment from Rifle, CO, that is rich with microbes in the genus *geobacter*.

In this sediment, it is well known that the community of anaerobic microbes will utilize acetate as an electron donor and subsequently reduce sediment-bound Fe(III) to Fe(II). In the presence of Fe(II),soluble, high oxidation state metal contaminants such as $Tc^{VII}O_4^-$ will be reduced to a low-solubility form such as $Tc^{IV}O_2$, immobilizing the contaminant as it precipitates onto sediment surfaces. At contaminated sites, it is common to inject electron donor solutions into wells dug deep into saturated subsurface sediment in order to drive this bioreductive process, but many questions still exist about the extent of influence these techniques have.

To provide insight into the mechanism of bioreductive processes, we have built 5.5 cm by 7.8 cm by 2.5 cm mesocosm as a simulation of a well amending sediment with acetate, using tracer levels of ^{99m}Tc-pertechnetate as a proxy for a metal contaminant flowing through this saturated system. The ratio of flow between simulated groundwater flow (across entire mesocosm) and 16 mM acetate (introduced 2.6 cm downstream of groundwater entrance) was approximately 20:1. Effluent water was measured for pH, dissolved O_2, Fe(II), sulfide, sulfate, and acetate concentrations.

The system was imaged in two ways: (1) using a pair of gamma-camera heads to measure ^{99m}Tc-distribution dynamically as ^{99m}Tc-pertechnetate was injected as a bolus into either the groundwater stream or the simulated well, or (2) using a PET camera to dynamically measure ^{11}C-acetate distribution injected as stated above. Concentration of radiotracer was also measured at both the inlet and outlet of the microcosm to gather breakthrough curves for each tracer and injection path. The mesocosm was frequently probed using both radiotracers at time points starting before acetate amendment, following amendment, during microbial buildup and through the iron reduction state.

^{99m}Tc imaging studies revealed that iron reduction only takes place downstream of the point of acetate amendment, presumably due to the growth of the redox-rich microbial community and resulting anaerobic local environment. ^{11}C-acetate imaging studies demonstrated acetate metabolism at both the boundaries of the microbial community buildup as well as potentially within the reductive zone. Ongoing work includes 16s ribosomal RNA analyses throughout the mesocosm, in addition to reactive transport modeling of the system.

Visualizing the Soil Carbon-Mineral interface: STEM-EELS Analysis of Soil Microaggregates

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Soil C accumulation and storage is an important contribution to the global C budget, with implications for C sequestration, atmospheric greenhouse gas levels, and climate, as well as maintenance of soil fertility. Interactions between soil organic carbon (SOC) and mineral surfaces are one process increasing SOC stability, but the chemical, physical, and biological mechanisms of SOC-mineral interactions are not confirmed. The combination of microscopic imaging of SOC spatial distribution with spectroscopic analyses allows for exploration of heterogeneous and complex interaction mechanisms at the SOC-mineral interface. Scanning Transmission Electron Microscopy (STEM) coupled with Electron Energy Loss Spectroscopy (EELS) is an emerging analysis technique for application to soils, with potential for very high-resolution visualization and chemical characterization of the SOC-mineral interface. We present preliminary EEL spectra for SOC reference compounds, and initial focused ion beam sample preparation of natural soil aggregates from model ecosystems with mineral-controlled SOC turnover. Development of STEM-EELS to elucidate SOC-mineral interaction mechanisms will serve to improve estimation of binding kinetics and stability, with application to the prediction and modeling of SOC dynamics.

Management Effect on Soil Organic Matter Distribution near Intra-Aggregate Pore Aggregate Structure as Determined by µCT images

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Soil organic matter (SOM) is an important soil quality that plays a major role in agricultural sustainability. SOM is known to positively affect soil aggregation, soil cation exchange, soil water holding capacity, and soil drainage in agricultural soils. In addition, SOM in soils is the major sink of atmospheric CO_2 in terrestrial settings. By increasing SOM in agricultural soils, climate change can be mitigated. Agricultural management affects the amount of SOM in agricultural soils. Tillage is one of the main influences on SOM from agricultural management. Another major component influencing SOM is duration, variety, and amount of vegetation and their inputs. Conventional tillage (CT) utilizes tillage and leaves fields exposed without cover for long periods of time, which allows more SOM decomposition by microorganisms to take place. Therefore, CT contains the lowest amount of SOM. Management that utilized cover crops as part of the rotation (O) uses cover year round, but still utilizes tillage, resulting in more SOM storage than CT. Natural vegetation (N) contains the amount of SOM believed to be near or at maximum storage capacity of a soil.

A lot of protection and storage of SOM is believed to take place within soil aggregates. However, detailed understanding of the mechanisms driving the intra-aggregate protection is still lacking. It is generally assumed that pore structure within aggregates is important for SOM storage, as pores determine access to carbon sources for microorganisms. Different pore size distributions affect how microorganisms can travel through an aggregate and, therefore, access SOM sources. This, in turn, determines utilization and possibly distribution of SOM within a soil aggregate.

Most techniques for soil analyses are destructive; however, the advent of computed microtomography (µCT) has allowed for *in situ* nondestructive analysis of soil aggregates visualizing intact intra-aggregate pore structure and its features. Images obtained from µCT are 3D gray scale images in which the gray scale values (GVs) correlate to structural components of the studied material. For soil samples, the important components influencing the image GVs patterns are differences in mineralogy, distribution of solid/void space, density, and presence and amount of SOM. Because SOM has a lower density than the mineral phase, it typically has lower GVs on the images. Our preliminary results indicated that intra-aggregate soil carbon is significantly correlated with image GVs. Here, we would like to build on this relationship to explore spatial patterns in the GVs of intra-aggregate solid material in relation to positions and characteristics of soil pores. We assume that the GV patterns will serve as an indirect indicator of SOM patterns. Our hypotheses are that O and N treatments will have more SOM closer to the pores, while CT management will have less SOM closer to the pores. The study objective is to examine the GV distribution around pores within aggregates from three different management types (CT, O, and N). Soil aggregates (n=32) had pores defined on the images using indicator kriging. Pixels at 0-5, 5-10, and 10-15 pixel lengths away from defined pores were then analyzed for average GVs for whole aggregates as well as 200 × 200 × 200 sections (n=96). Average GVs were compared to the average GVs of the entire image without pores to account for any GV differences between images. Because the mineralogy of all aggregates is very similar, lower GVs indicate more SOM and vice versa. Results show that GVs tend to be lower for N treatment and higher for CT treatments, with the lowest GVs occurring at the 5 pixel interval for all treatments.

Monitoring of Nitrous Oxide Emissions during Soil Drying with X-ray Computed Tomography

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Nitrous oxide (N_2O) has long been recognized as playing a role in stratospheric ozone depletion and global warming. Soils are a major source of N_2O, as they account for 60% of natural N_2O sources and 60% of anthropogenic sources (Ciais et al., 2013). Water in soil is known to be a key factor for controlling N_2O emissions, because N_2O is mainly produced by gentrification in anoxic environments. Moreover, the quantity and the distribution of water-filled pores at a given pressure head, an element of the soil structure, appear to play a role in N_2O production and emission processes, since they regulate flow of water and gases.

In this study, we investigated the effect of wetting and drying cycles on the N_2O emissions of a soil sample, and also studied the effect of water hysteresis. The experiment involved controlling the hydric status of a soil sample with a multistep outflow system while measuring N_2O emissions. An undisturbed soil core (13.2 cm inner diameter, 7 cm height) was first saturated for three days, and then submitted to a –100 hPa pressure at its bottom. The wetting and drying cycle was applied two times (C1 and C2 cycles). Both the water content and water potential were continuously monitored during the experiment. Nitrous oxide emissions were measured using the closed-chamber technique. The soil core was scanned with X-ray computed tomography (resolution 300 µm) one time at saturation and seven and nine times for C1 and C2, respectively, during the drying phase. Image processing was realized with the ImageJ software (Rasband, 1997-2014) and the C library QuantIm v.4 (Vogel, 2008). The air phase was separated from the soil matrix and the water phase using the k-means segmentation method. Quantitative and qualitative indicators of the pore network were calculated from the segmented images: the volume of macropores and the Euler number. The Euler number allows characterizing the connectivity of the pore space. It classifies the pore network as unconnected when it is positive, and unconnected when negative.

Nitrous oxide emissions were lower during C2 than during C1, both for the wetting and the drying phases. Fluxes were measured to be 9.4 and 0.1 mg N m^{-2} d^{-1} at the end of the C1 and C2 wetting phase, respectively. Fluxes increased quickly after the beginning of the drying phase to reach a peak ~5 hours after the beginning of the soil drying. Maximum N_2O fluxes were 55.1 mg N m^{-2} d^{-1} for C1, and 19.1 mg N m^{-2} d^{-1} for C2. Maximum N_2O fluxes were reached at ~ –45 cm water column, when pores with radius >57 µm were drained, according to the Jurin-Laplace law. Air-filled pore volume increased rapidly during the first hour of drying, and then increased more slowly. The Euler number, slightly higher than zero during the whole experiment, reveals that the segmented pore network was not entirely connected. Emissions may have occurred from the soil upper part connected to the atmosphere. The connectivity of the air phase was higher at C2 than at C1. The soil matrix, drier for C2 than for C1, revealed a higher anoxia level during C1 than during C2, and consequently explained higher N_2O fluxes during C1.

The results of the present study are consistent with the hypothesis that N_2O has been entrapped both in the gaseous and the liquid phases during wetting, and that the increase in the gas diffusion through the increase in the connectivity to the soil surface was responsible for the N_2O peaks observed during drying. This study highlighted the need to find and measure dynamic indicators of the soil structure, to enhance our understanding of the dynamic nature of N_2O emissions by soils.

Soil Microbial Community Shifts in Response to Soil Thermal Insulation and Vegetation Change in Moist Acidic Tundra of Northern Alaska

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The effects of rising temperatures on ecosystems remain largely unknown and are an active area of research. In temperate systems, plant species often respond directly to climate forcing factors causing complex cascading effects in ecosystem carbon and nutrient cycling. Similarly, in the Arctic tundra, shifts in aboveground species composition and distribution have been observed in response to soil warming and its resulting increases in active layer depth. Initial abiotic changes provide soil microorganisms access to previously unavailable soil organic matter (SOM) via thawing soils, increasing soil microbial decomposition and nutrient mineralization rates, and resulting in soil organic carbon loss and increased nutrient availability.

Here, we examine how microbial communities respond to increases in soil thermal insulation and vegetative change caused by the accumulation of winter precipitation at a snowfence installed in 1994 at Toolik Field Station, Alaska. We hypothesize that soil microorganisms are eliciting the plant response through the release of nutrients under warmer conditions, providing a competitive advantage to N-rich woody species, such as dwarf birch and diamond-leaf willow, over herbaceous species such as cottongrass tussock. Changes in plant litter (and thus soil chemistry) and increasing NPP may contribute to SOC re-accumulation and alter microbial community composition. Bacterial/fungal phylogenies and relative abundances from soils collected in August of 2012 were determined by V4 16S rRNA and ITS amplicon sequencing of extracted DNA. We found significant shifts in relative abundances of bacteria and fungi between snow depth treatments (deep, intermediate, low) and soil horizons (organic, transition, mineral), most notable of which include in a decrease in *Verrucomicrobia* of the family Chthionobacteraceae (known to be a facultative aerobic heterotroph able to grow on saccharide components of plant biomass and possibly capable of methanotrophy), an increase in Deltaproteobacteria in the deep treatment zones, a decrease in Alphaproteobacteria with increased soil depth, and a marked increase in Chloroflexi of the family Anaerolinaceae (a facultative anaerobic green nonsulfur bacteria found in a wide range of habitats) in the deep treatment zones and mineral layers. Other interesting results include the presence of two novel, uncultured phyla of bacteria, AD3 (phylogenetically related to green nonsulfur bacteria), which was found in mineral layers across all treatments, and OP8 (yet to be characterized), found only in the mineral layers of the deep snow depth treatment.

These shifts in microbial community composition in response to simulated future climate conditions (i.e. increased winter snow depth) suggest a potential shift in the functional capacity of the community, which may alter carbon and nutrient cycling in the ecosystem and facilitate observed plant community shifts.

Plant Invasions Are Associated with Changes in Root-Zone Fungal Communities

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The importance of interactions among plants, soil, and microbes is well acknowledged. Although it is observed that plant species alter the natural ecology, few studies have documented the changes that are associated with the colonization and establishment of invasive plants. We aimed to understand whether the fungal communities in the root zone were different between paired sets of three different invasive and native plants. Towards this end, we sampled five replicates from the root-zone soil (15 cm deep) along a 30 m transect at three sites growing the invasive plants: *Microstegium vimineum, Rhamnus davarica* and *Ailanthus altissima*. Reference sites with established native vegetation on adjacent soil transects were sampled identically. To identify the fungal community composition and structure associated with each invasive and reference plant, Illumina MiSeq sequencing of the Internal Transcribed Spacer region of rRNA genes were analyzed using QIIME. Overall, the results showed that soils that were impacted by invasive plants had fungal community composition and structure that differed from those of soils with reference plants. *Microstegium vimineum* was associated with the greatest changes relative to reference vegetation. The data support the hypothesis that invasive plants alter fungal communities in their root zones.

Long-Term and High-Frequency Nondestructive Monitoring of Soil-Water Stable-Isotope Compositions in the Laboratory

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In soils, the isotope compositions of water (δ^2H and $\delta^{18}O$) provide qualitative information about whether water has only infiltrated or has already been re-evaporated since the last rainfall event, or about the location of the evaporation front. From water stable-isotope profiles measured in soils, it is also possible, under certain assumptions, to derive quantitative information, such as soil evaporation flux and the identification of root-water uptake depths. In addition, the fate and dynamics of water stable isotopologues have been well implemented into physically based soil–vegetation–atmosphere transfer (SVAT) models (e.g., Hydrus 1D, SiSPAT-Isotope, Soil–Litter iso, TOUGHREACT) and have demonstrated their potential.

However, the main disadvantage in the use of stable isotopes in soil water studies is that, contrary to other state variables (e.g., water content and tension) that can be monitored over long periods (e.g., by time-domain reflectometry, capacitive sensing, tensiometry or micro-psychrometry), stable-isotope compositions are analyzed following destructive sampling, and thus are available only at a given time. As a consequence, there are important discrepancies in time resolution between soil-water and stable-isotope information which greatly limit the insight potential of the latter.

Recently, a novel technique based on infrared laser absorption spectroscopy was developed that allows simultaneous and direct measurements of δ^2H and $\delta^{18}O$ in water vapor, which constitutes a major breakthrough in stable isotope analysis. Many applications can be found in the literature for varying temporal and spatial scales. Here, we present a non-destructive method for monitoring soil liquid water δ^2H and $\delta^{18}O$ by sampling and measuring water vapor equilibrated with soil water using gas-permeable polypropylene tubing and a cavity ring-down laser absorption spectrometer.

Three acrylic glass columns (diameter = 11 cm, height = 60 cm) were (i) equipped with temperature and soil-water probes in addition to gas-permeable tubing sections at eight different depths (1, 3, 5, 7, 10, 20, 40, and 60 cm), (ii) filled with pure quartz sand (grain size < 1 mm), and (iii) saturated from the bottom up to the surface. Finally, they were installed on weighing balances and let dry for 250 days.

Each day, soil-water vapor δ^2H and $\delta^{18}O$ were measured sequentially for each depth by (i) purging the soil water vapor sampled in the tubing sections with dry synthetic air, (ii) diluting the obtained gas mixture again with dry synthetic air, and (ii) analyzing it with a cavity ring-down laser spectrometer. Soil liquid water δ^2H and $\delta^{18}O$ were then inferred from the values in the vapor by assuming thermodynamic equilibrium between liquid and vapor phases in the soil, which we could previously demonstrate to exist.

The experimental setup allowed following the evolution of the soil-water δ^2H and $\delta^{18}O$ profiles, which developed as a result of isotope convective capillary rise and back-diffusion of the stable isotope excess at the soil surface due to fractionating bare-soil evaporation, with unprecedentedly high temporal resolution. Results show the formation over time of typical and previously well-documented logarithmical shaped δ^2H and $\delta^{18}O$ profiles. As the soil dried out, we could also show for the first time the increasing influence of the isotopically depleted ambient water vapor on the isotopically enriched liquid water close to the soil surface (i.e., atmospheric invasion). Finally, the setup provided (i) insight into the dynamics of the evaporation front in the soil by identifying the depth of maximal δ^2H and $\delta^{18}O$, and (ii) values of soil evaporation fluxes from the confrontation of the δ^2H and $\delta^{18}O$ profiles with analytical formulations for water stable-isotope transport in the soil.

The Effect of Compost on Carbon Cycling and the Active Soil Microbiota

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Rangelands cover an estimated 40-70% of global landmass, approximately one-third of the landmass of the United States and half of California. The soils of this vast land area have high carbon (C) storage capacity, which makes it an important target ecosystem for the mitigation of greenhouse gas emission and effects on climate change, in particular under land-management techniques that favor increased C sequestration rates. While microbial communities are key players in the processes responsible for C storage and loss in soils, we have barely shed light on these highly complex processes, in part due to the tremendous and seemingly intractable diversity of microbes, largely uncultured, that inhabit soil ecosystems.

In our study, we compare Mediterranean grassland soil plots that were amended with greenwaste compost in a single event 6 years ago. Subsampling of control and amended plots was performed in depth increments of 0-10 cm. We present data on greenhouse gas emissions and budgets of carbon, nitrogen, phosphorus, and micronutrients in dependence of compost amendment. Changes in the active members of the soil microbial community were assessed using a novel approach combining flow cytometry and 16S tag sequencing disclosing "*who is active.*" This is the first study revealing the nature of actively metabolizing microbial community members linked to the geochemical characteristics of compost-amended soil.

Metabolomics Approaches To Understand Microbial Carbon Cycling in Grassland Soil

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The cycling of soil organic matter (SOM) by microorganisms is a critical component of Earth's carbon cycle, but remains poorly understood. Of vital importance is how the distribution of carbon between the atmosphere and the subsurface will change in response to altered rainfall, temperature, and vegetation patterns. In this project, we investigate how altered rainfall impacts the dynamics of carbon stored in grassland soil using a long-term ecological research site in California (the Angelo Coast Range Reserve) that features an ongoing experimental manipulation of water inputs to mimic shifting precipitation regimes that are relevant to climate change scenarios. Here, we establish a simple soil extraction and metabolomics workflow that will enable rapid comparison between samples collected at various timepoints during rainfall manipulation and at different depths.

To release metabolites from microorganisms and obtain a measurement of total SOM, soil was fumigated with chloroform vapor while unfumigated soil was used as a measure of extracellular compounds. A series of extractants were tested (aqueous vs. organic solvents) and extracts analyzed by gas chromatography/ mass spectrometry. In total, 60 metabolites were identified, with fumigation having a significant effect on the range and intensity of metabolites. Sugars (fructose, glucose, trehalose, sucrose) were among the most abundant, followed by sugar alcohols, fatty acids, dicarboxylic acids, sterols, nucleobases, osmolytes and many other metabolic intermediates. Water was one of the most effective extractants in terms of the number and range of metabolites detected. The inclusion of organic solvent facilitated the extraction of fatty acids and sterols.

This study presents a simple SOM extraction and metabolomics workflow that will be combined with genomics, proteomics, and transcriptomics to understand how the grassland ecosystem will respond to future climate change.

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Advanced Characterization of Soil Organic Matter Using Ultra-High-Resolution Mass Spectrometry

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The focus on ecosystem stress and climate change is currently relevant as researchers and policymakers strive to understand the feedbacks between soil C dynamics and climate change. Successful development of chemical/molecular profiles that link soil microbiology with soil carbon (C) to ascertain soil vulnerability and resilience to climate change would have great impact on assessments of soil ecosystems in response to global climate change. Additionally, better understanding of the dynamics of soil organic matter (SOM) plays a central role to climate modeling, fate and transport of carbon, and mineral SOM interactions. Current methods used to characterize organic matter in the solid and aqueous phases lack the molecular and elemental detail that is necessary to develop predictive, mechanistic models of the key processes that operate in the belowground ecosystem. However, recent advances in the area of ultrahigh resolution mass spectrometry (UHR MS) have improved this situation. The use of UHR MS, in particular Fourier transform ion cyclotron resonance MS (FT-ICR MS), usually coupled with electrospray ionization (ESI), has enabled the examination of molecules directly from mixtures with ultrahigh mass resolution and sub-ppm mass accuracy. The use of FT-ICR MS has, however, been limited to dissolved organic matter (DOM) mixtures collected from rivers, lakes, and estuaries. Here, we demonstrate how UHR MS can be used to gain information about the molecular composition of soil organic matter.

EMSL's extensive expertise and capabilities in UHR MS proteomics were leveraged to develop extraction protocols for the characterization of carbon compounds in SOM, thereby providing the chemical and structural detail needed to develop mechanistic descriptions of soil carbon flow processes. Solvent extractions are the most commonly used procedures to prepare extracts from soil, due to their ease of use, efficiency, and wide applicability. Our experiments have allowed us to identify thousands of individual compounds in complex soil mixtures with a wide range of C content, representing diverse ecosystems within the USA. This UHR technique generated large databases of chemical formulas for individual samples, which could be searched for specific compounds and compound classes, or integrated across the entire dataset to summarize the molecular characteristics of SOM (e.g., aromaticity, elemental ratios, and degree of unsaturation). Moreover, our experiments have shown that the yield of the chemical extraction was dependent on (1) the type of solvent used and its polarity, (2) sample-to-solvent ratios and (3) the chemical and physical nature of the samples, including their origins. Hexane, a nonpolar organic solvent, was efficient in extracting lipid and lipid-like compounds regardless of soil origin or organic carbon %. For samples with high organic carbon %, acetonitrile extracted a wide range of compounds characterized with high O/C ratios, characterized as polyphenolic compounds that were not observed with methanol extraction. Soils extracted with pyridine showed a similar molecular distribution to those extracted by methanol.

The results from these experiments show that solvent extraction followed by UHR MS is a promising tool to understand the dynamics of SOM. The information gained from this study has been used on different user proposals assessing the sensitivity of soil carbon decomposition and feedbacks to climate change. We present examples of several of these studies and demonstrate its potential in several studies involving the simulated change or ecosystem gradients.

Noninvasive Imaging of CO_2 Uptake in Biological Soil Crusts

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Biological soil crusts (BSCs) play many important roles in the ecosystems of arid and semi-arid regions worldwide. One such role is carbon fixation, where photosynthetic microorganisms such as cyanobacteria can play a key role. In these systems, carbon fixation is strongly regulated by water availability; however, following periods of extreme drought, photosynthesis is known to reactivate within minutes of a rainfall event. These pulsed-activity events represent "hot moments" of biological activity in these systems. However, BSCs are known to have a high degree of spatial heterogeneity in both distribution and function, with "hot spots" potentially contributing disproportionately to photosynthetic activity. Currently there are insufficient scientific tools spanning the micro- and mesoscales to quantify such heterogeneity. Using 11-carbon labelled CO_2, we have performed a set of experiments mapping CO_2 fixation using positron emission tomography, measuring heterogeneity in carbon uptake at the millimeter scale under various environmental conditions.

Experiments consisted of tracking CO_2 uptake in BSCs following exposure to radiolabelled $[^{11}C]CO_2$ gas in a sealed chamber and subsequent measurement and imaging of radiolabel retention spatially across the surface of BSCs using a positron emission tomography (PET) camera. Using this highly sensitive, nondestructive radiotracer technique allowed for multiple measurements between each of three wetting events over 2.5 extended diel (day/night) cycles in order to investigate the role of water and light on the regional uptake of CO_2. With each PET experiment, photographs of BSCs were also taken and quantitatively analyzed for local "green" levels as an index of cyanobacterial (chlorophyll) surface density, and quantitative comparisons made between these images and $[^{11}C]CO_2$ fixation images.

We hypothesized that regions of the crusts with a visibly higher concentration of cyanobacterial filaments would have greater $[^{11}C]CO_2$ uptake. The results support this hypothesis as in general, the pattern and magnitude of $[^{11}C]CO_2$ uptake matched that of cyanobacterial surface density. This relationship was strongest following a simulated rainfall event under light; however, a decoupling between cyanobacterial surface density and $[^{11}C]CO_2$ uptake could be observed (as expected) without light and following an extended drying. $[^{11}C]CO_2$ uptake in heat-killed controls also suggests a minor contribution of abiotic pathways for CO_2 uptake relative to biological pathways.

In conclusion, we present this technique to demonstrate that application of radioisotope imaging to the study of BSCs represents a valuable tool for defining millimeter-meter scale biological functional heterogeneity in soils. We propose that modified protocols could be used to quantify the rate of CO_2 fixation through photosynthesis or other metabolic processes, as radioisotope imaging is well suited for longitudinal, noninvasive mapping and quantification of dynamic biochemical processes.

3D Characterization of Soil Aggregates: New Opportunities from Submicron-Resolution Synchrotron X-ray Microtomography

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In soil science, the study of "hot spots" is gaining increased attention. Such research seeks to address why soils exhibit discrete zones of high biological activity at small spatial scales. The mechanisms responsible for hot-spot formation and maintenance are open questions currently being tackled from many different perspectives, including spatial mapping of localized biological activity, but also by attempting to correlate physical and chemical heterogeneities related to the development of these hot spots (e.g., controls related to nutrient availability, microbial micro-habitat, and bulk transport). This study focuses on the spatial/microstructural aspect of this problem, with the goal of determining the relationship between soil aggregate structure, pore-network geometry, and the formation of hot spots. As a first objective, we propose a protocol for the analysis of single soil aggregates, in the sub-millimeter-size range, using synchrotron X-ray microtomography (SXR-μCT) with submicron resolution. Our fundamental goal is to define associations between the morphometric parameters obtainable via SXR-μCT datasets with the chemical and biological properties of soil aggregates.

As a demonstration of the utility of SXR-μCT for characterizing the physical environment in which microbial activity is regulated in soils, we have chosen aggregates from two soils with markedly different organic matter content: individual ~200 μm aggregates, one mostly inorganic in nature, from the Konza Prairie (Kansas, USA), and one mostly organic from the Barrow Environmental Observatory (Alaska, USA) were examined. The measurements were carried out at Beamline 8.3.2 at the Advanced Light Source (Lawrence Berkeley National Laboratory). Aggregates were measured in a sealed glass capillary, obtaining a nominal 325 nm voxel size for the reconstructed dataset, and a submicron effective resolution. A single distance phase-retrieval algorithm has been used to enhance the contrast of the different phases, a necessary step to provide higher quality raw reconstructed data and simplifying the segmentation process.

Several novel analysis techniques have been developed to characterize the soil aggregates in a quantitative fashion. First, we developed a procedure to separate the "inner pore space" from the "air" surrounding the aggregate. Simple (gray scale based) segmentation does not work for this task, and a series of morphological operations and masking procedures were necessary to separate the air inside and outside the sample. We highlight this approach as it enables more accurate calculation of volume fractions (true pore space and solid material volume percentages) within aggregates. Furthermore, through morphological operators and pore space skeleton calculation and analysis, we have been able to obtain the size distribution (and position) of the openings on the surface of the aggregates. This is key to determining how accessibility of the inner space (i.e., larger pores) of the aggregates to microorganisms relates to physical protection of carbon from decomposition. Following this concept, we have been able to calculate which parts of the pore space are *geometrically* accessible from the outside of the sample to different microorganisms based on their size, highlighting aggregate regions with high porosity but that are inaccessible to large-to-medium-sized microorganisms. Other more conventional morphometric analysis techniques have been used as well, including local thickness, characterization of pore-size distributions, and skeleton analysis to quantify the complexity and the connectivity of the pore space. Our results show that the aggregates display significant differences from the morphometric point of view, and that SXR-μCT can provide significant *quantitative* information to the soil scientist also at the micro-nanoscale.

Lastly, 3D printing of the samples has been carried out (and will be presented) to help with the visualization of the soil aggregates, an important approach to communicating the topic of microbial-scale heterogeneity in soils.

Reactive Transport Modeling Parameterization Using Geophysical Datasets

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Developing an understanding of biogeochemical dynamics in terrestrial environments requires consideration of a broad range of processes that occur across disparate space and time scales. In this presentation, we describe the development and implementation of a Bayesian approach to integrate point measurement, Time-domain Induced Polarization (TDIP) data collected within a floodplain located near Rifle, CO. This site, located next to the Colorado River, is the focus of a new DOE project aimed at developing a predictive understanding of how the subsurface microbiome affects biogeochemical watershed functioning, how watershed-scale processes affect microbial functioning, and how these interactions co-evolve with climate and land-use changes. This presentation will describe how spatially extensive geophysical measurements can be used to identify controls on and improve predictions of terrestrial environment functioning.

Inversion of the TDIP data enabled obtaining images of complex resistivity (CR), which provide information about the conductivity and the polarization properties of the subsurface. As demonstrated in previous studies at the site, the images of the real component (conduction properties) are related to hydrogeological properties (e.g., changes in lithology, saturation); whereas images of the imaginary component (polarization) are mostly associated with the occurrence of metallic minerals due to microbial activity. We relied on the TDIP data to delineate naturally reduced zones (NRZs), which may serve as “hotspots” for biogeochemical processes within the floodplain. Comparison of the CR images to co-located wellbore data showed that the NRZs have a distinct distribution of the complex-resistivity phase images, well separated from that in non-NRZs. To estimate the spatial distribution of NRZs, we developed a Bayesian hierarchical model that can integrate SIP and well log datasets in a consistent manner. Markov-chain Monte-Carlo methods were used to compute a probability field of NRZ and provide random fields for the stochastic simulations of reactive transport. The geophysically identified NRZ distribution was used in reactive transport modeling, the results of which showed a geochemical concentration pattern consistent with the observations at the site.

Images of the real component of the complex resistivity were used to estimate the depth of the hydrostratigraphic interfaces of the artificial fill and Wasatch formation underlying the aquifer. We obtained the threshold resistivity values at the interfaces using co-located wellbore datasets, and then used a kriging method with a variable data-error covariance so that we could integrate the wellbore and resistivity datasets consistently. The estimated interfaces turned out to be significantly different from the previously estimated ones, based solely on sparse wellbore data, capturing more detailed heterogeneity. These interfaces were also used to parameterize the reactive transport models. The modeling results suggested that the concentrations were affected particularly by the Wasatch thickness, due to its control on mixing.

Nitrogen Cycling and Soil Fungal Communities along Gradients of Forest Composition Factors and Age in Regenerating Tropical Dry Forests

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Soil nitrogen (N) cycling in secondary tropical forests is driven by multiple interacting biogeochemical drivers, including abiotic factors, plant and microbial community composition, and land-use history. Here, we explored how plant associations with mycorrhizal fungal symbionts influence soil N cycling at the ecosystem scale. Ectomycorrhizal fungi (ECM) can access organic nutrients whereas arbuscular mycorrhizae (AM) mainly exploit inorganic nutrient pools, and these contrasting processes may influence the relative importance of organic versus inorganic N cycling at the stand level. Therefore, we hypothesized that effects of plant community composition on soil N cycling would be mediated through fungal community composition.

To quantify the relative importance of abiotic factors, plant and microbial community composition, and land-use history on soil N cycling, we studied three separate forests in Costa Rica that differ in stand age and the relative abundance of ECM trees: Santa Rosa oak forest (high percentage of ECM trees), Santa Rosa tropical dry forest (low percentage), and Palo Verde tropical dry forest. We sampled soils within 8 subplots in each of eighteen 0.1 ha plots across the three forest stands. In addition to determining microbial biomass, inorganic N pool sizes, nitrogen mineralization rates, and the activities of microbial extracellular enzyme that mediate organic N depolymerization, we also characterized fungal community structure through amplicon-based high-throughput sequencing.

Fungal community composition was extremely diverse, with ~8,000 fungal taxa identified. Most variation in both fungal community composition and N cycling rates occurred at the subplot scale. However, there were broad patterns in community composition and N cycling across the three forest types, associated with a significant shift in the relative abundance of mycorrhizal fungi. In forests growing on poorer soils (i.e., the oak forest), mycorrhizae were more abundant relative to free-living fungi, microbial biomass C:N was higher, and N mineralization rates tended to be lower. Both ECM and AM mycorrhizal community composition were linked with N cycling rates, and saprotrophic community composition explained a small proportion of the variation in N fluxes and pools. We conclude that fungal communities are structured at relatively small spatial scales and are sensitive to plant community composition and soil nutrient availability. In addition, it appears that soil N cycling is more strongly influenced by relative abundance of fungal functional groups than the identity of fungal species.

Advanced *In Situ* Measurement of Soil Carbon Content Using Inelastic Neutron Scattering

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Measurement and mapping of natural and anthropogenic variations in soil carbon stores is a critical component of any soil resource evaluation process. Emerging modalities for soil carbon analysis in the field is the registration of gamma rays from soil under neutron irradiation. The inelastic neutron scattering (INS) of fast neutrons (with energy around 14 MeV) on carbon-12 nuclei produces gamma rays with energy of 4.43 MeV and the registration of this gamma flux can be directly used for determination of carbon contained in soil. The INS method has several advantages over other methods of carbon determination like dry combustion, laser induced breakdown spectroscopy, or mid- and near-infrared reflectance spectroscopy. The INS method is nondestructive, requires no sample preparation, and analyzes a large soil volume in a single measurement. Due to these features, the INS method can be applied for *in situ* routine soil carbon determination.

Currently this method is in development at the USDA-ARS National Soil Dynamics Laboratory. Previous findings from Brookhaven National Laboratory (Wielopolski et al., 2000-2012) were utilized to facilitate the physical construction and electronic requirements of a mobile INS system (MINS) for carrying out routine field measurements. The MINS power system (consisting of four 12V batteries with 105Ah, a DC-AC inverter, and a charger) is capable of powering a MP320 neutron generator, a neutron detector, three 12.7 cm × 12.7 cm × 15.2 cm scintillation NaI (Tl) detectors with corresponding electronics, and the laptop computer that controls the neutron generator, detectors, and data acquisition. The MINS was designed to operate on a platform that can be maneuvered by tractors or all-terrain vehicles over any type of field.

Using MINS, measurements of the 4.43 MeV gamma peak were conducted at 28 field sites. For carbon in the 0–30 cm soil layer, a comparison of the corrected 4.43 MeV peak (i.e., overlapping gamma peaks due to other carbon-12 nuclei and processes) with chemical analysis (dry combustion method) showed a direct correlation.

The MINS was operated in two modes, pulse and continuous. Comparison of these modes for carbon measurement accuracy was conducted using sand/carbon mixtures (40 cm × 40 cm × 20 cm) representing various carbon percentages. Since the measurement time in the continuous mode was half that of the pulse mode with the same accuracy, the continuous mode was preferable for routine soil carbon measurements. To further access the possibility of *in situ* carbon measurement in the continuous mode, MINS was calibrated using 1.5 m × 1.5 m × 0.6 m boxes filled with soil mixtures of known carbon percentages. Collectively, this information will be used in future field studies to evaluate the ability of MINS to obtain *in situ* measurements of soil carbon.

Theme 3: Modeling of Soil Systems

Why Is There Universality in Saturation-Dependent Transport?

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Most forms of transport in soils show essentially the same dependence on the volume fraction of the conducting phase(s). Examples include relative permeability of both wetting and nonwetting phase fluids, diffusion of both wetting and nonwetting phase fluids, electrical conductivity, and thermal conductivity. This universal behavior seems counter-intuitive to soil scientists, because (1) different forms of transport have different dependencies on the pore radius, (2) saturation dependence has an inherent asymmetry—wetting fluids preferentially occupy small pores while nonwetting fluids compete for the large pores, and (3) the solid phase has higher thermal conductivity than either fluid phase, but it is a barrier to fluid flow. So the overwhelming *experimental* evidence for this universal behavior presents a conceptual challenge: why is there universality where we have always seen diversity?

The *theoretical* evidence for universality, grounded in percolation theory, reveals an underlying structure in the conducting pathways through disordered materials. Taking hydraulic conductivity as an example, soil physics has traditionally focused on geometry (for example, pore size). But because individual large pores do not typically span the entire soil, flowpaths must also include smaller pores. The topology (connectivity) of the flowpaths therefore becomes an important constraint and dominates the $K(\theta)$ curve at low water contents. Topology likewise dominates the other forms of transport, to an even greater extent than for hydraulic conductivity: even in the face of different pore-scale dependencies, the asymmetry of wetting / nonwetting pore occupancy, and the high versus zero conductivity of the solid phase, the universality indicated by percolation theory gives a single functional form for saturation-dependence transport.

The unexpected emergence of a universal behavior, where soil science has always seen unrelated, disparate phenomena, suggests a fundamental rethinking of how we approach transport.

Effective Permeability in Multi-Component Porous Media: Lattice-Boltzmann Model and Effective Medium Approach Applications

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Porous media e.g., soils and rocks, are complex and typically heterogeneous mixtures built up of two or more components with intrinsic permeabilities depending on pore shape and surface area, tortuosity, connectivity, etc. In such mixtures, the effective transport coefficient (e.g., permeability) of the mixture is a combination of the transport coefficients (permeabilities) of the individual components. In disordered random composites, the effective permeability can be predicted by different methods. Here, we present applications from modern techniques, such as Lattice-Boltzmann model (LBM) and effective medium approach (EMA). The LBM is a computational fluid dynamic method with a remarkable ability to simulate flow and transport based on statistical mechanics. The EMA is an analytical treatment for the prediction of the effective transport coefficients of disordered composites. Advantages and disadvantages of each model are discussed in detail. In addition, we compare the predictions by the applied methods with the experimental data measured in lab

Theoretical Relationship between Surface Fractal Dimension and Water Content Measured at Permanent Wilting Point: Adsorbed Water Films Effect

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Surface fractal dimension D_s quantifies the pore-solid interface structure in porous media. In this study, we propose a theoretical framework to investigate the relationship between the surface fractal dimension D_s and the water content remaining in the medium at 1500 kPa tension, θ_{pwp}. Using concepts from adsorbed water films, and van der Waals and electrostatic forces, we present a logarithmic function relating D_s to θ_{pwp}. Our model, similar in form to the relationship proposed experimentally by Ghanbarian-Alavijeh and Millán (2009), provides a physical interpretation for the two empirical coefficients in their expression. We also examined the sensitivity of the Hamaker constant and found that it does not influence the surface-fractal-dimension predictions considerably. We also found that when the water-film thickness is underestimated, the surface fractal dimension D_s is overestimated, which is consistent with the Mandelbrot definition of path lengths on geometrical fractals. For the purpose of practical prediction of surface fractal dimension using the model developed in this study, we used 172 soil samples from five databases available in the literature. We assumed adsorbed water thickness equal to 1 nm for both van der Waals and electrostatic films. Then, for each soil sample, we used the measured porosity and θ_{pwp}, and the calculated air entry values to predict the surface fractal dimension. We found that the predicted D_s values agree very well with those calculated from the soil-water-retention measurements.

FLOGing Data To Link Carbon and Nitrogen Cycling from Organic Matter Additions to Agroecosystems

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A continuous, nonlinear model (FLOG-CN) of carbon mineralization and nitrogen mineralization-immobilization with respect to time was developed that successfully reproduced the complex CO_2-C and SMN dynamics for a collection of 76 paired C and N datasets. The FLOG-C model separates CO_2-C evolution into two pools that are separated in time: a first-order exponential pool representing highly labile C, and a logistic pool representing what we suggest is a complex form of C that is acted on by depolymerizing enzymes before mineralization. Given that the depolymerization of complex substrates has also been recognized as a likely rate-limiting step in nitrogen mineralization, and that soil nitrogen transformations under aerobic conditions are performed by organisms that respire CO_2-C, we propose using the time-separated CO_2-C pools to describe soil mineral nitrogen (SMN) dynamics. Nitrogen dynamics are coupled to CO_2-C evolution by assuming that nitrogen can either be mineralized or immobilized according to microbial demand during the decomposition of both the labile and polymerized pools, resulting in the FLOG-N model. In some cases (decreases in cumulative CO_2-C or initial lag phase in C dynamics during low incubation temperature), the model was not able to reach convergence or produced unrealistic parameter estimates. Application of the model to 76 diverse C and N datasets showed that incorporating latency into the model of C mineralization, and using C to drive N dynamics, allows heterogeneous data from many different soil amendments to be described by the same model. We successfully modeled complex CO_2-C and SMN dynamics of widely different shapes and from a variety of soil amendments containing plant and animal residues. The re-interpretation of these datasets with the FLOG-CN models improved the quantitative analysis of C and N dynamics, yielding new insights into how amendment characteristics and experimental conditions influence the timing and quantity of C and N mineralized. Model parameters were responsive to varying soil characteristics (pH, C, N, C:N), amendment N:C, amendment rate, incubation temperature, and N additions. Stepwise regression was used to predict model parameters using metadata available for 56 of these datasets. Significant linear relationships were developed to estimate model parameters independently, using measured system properties or other model parameters that could be independently estimated. Estimates of C and N dynamics both fell along a 1:1 line, indicating that the model parameters could be adequately described by the measured properties, but the available metadata was not able to describe C dynamics with high precision. Nitrogen mineralization-immobilization was strongly related to amendment N:C, and switched between the two processes at an amendment N:C between 0.077 to 0.085 (C:N between 11.7 to 12.9).

We believe that the modelling approach described here will allow quantitative and objective comparisons of diverse C and N datasets that have been hindered by subjective descriptions in the past.

Saturation Dependence of Transport in Soils: Modern Theories

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It is an axiom of physics that linear response theory is highly constrained, while nonlinear response is not. Thus, ohmic conductivities are easy to calculate, or at least represent, in terms of the Kubo-Greenwood formula, but nonohmic terms, especially in disordered systems, have no such formalistic guidance. It is also well-known that calculations of nonlinear response have little chance of success when the physics of the system is not well enough known to calculate the linear response. Here, we report that the traditional linear response equations of soil physics are inconsistent, inaccurate, and have no relationship with physics. However, we can calculate hydraulic and conduction properties of such media accurately if we use methods appropriate to disordered systems. These methods are percolation and effective medium theories. Applying these theoretical approaches consistently allows us to predict electrical and thermal conductivity, air permeability, and solute and gas diffusion coefficients as functions of saturation. Indeed, these properties are all given in terms of the same universal function and can be put on the same graph. We are also able to predict the delivery of solutes and chemical reaction rates as a function of soil saturation. Ability to predict the effects of (for example) biota on moisture content and chemical composition, as well as the effects of moisture content on flow and solute movement, will ultimately enable us to predict successfully the nonlinear interactions of an abiotic medium and biota in producing a soil. Techniques that ignore these advances may not make such successful predictions, and will only induce us to develop an enormous range of ad hoc parameters and hypotheses.

Trait-based Approaches to Modeling Microbial Biogeochemistry from Terrestrial to Aquatic Ecosystems

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Currently, there is uncertainty in how climate or land-use-induced changes in hydrology and vegetation will affect subsurface carbon flux, the spatial and temporal distribution of flow and transport, biogeochemical cycling, and microbial metabolic activity. Here, we report on the initial development stages of a Genome-Enabled Watershed Simulation Capability (GEWaSC), which will provide a predictive framework for understanding how genomic information stored in a subsurface microbiome affects biogeochemical watershed functioning, how watershed-scale processes affect microbial function, and how these interactions co-evolve. This multiscale framework builds on a hierarchical approach to multiscale modeling, which considers coupling between defined microscale and macroscale components of a system (e.g., a catchment being defined as macroscale and biogeofacies as microscale). The multiscale framework is based on an object-oriented, modular software design that couples individual process models (e.g., biogeochemistry, microbial function). Initially, we are focusing on biogeochemistry within the Rifle floodplain system, a component of the greater Colorado River system. At the floodplain scale, our model schema considers microbial competition and activity in discrete zones (biogeofacies) identified using a combination of biological, chemical, and geophysical approaches. These zones include surface soils with vegetation, the vadose zone and capillary fringe, and naturally reduced zones with buried organic material.

We also report our initial progress in the development of a trait-based modeling approach within a reactive transport framework that simulates coupled guilds of microbes. Guild selection is driven by traits extracted from, and physiological properties inferred from, large-scale assembly of metagenome data. Metagenome information is also used to complement our existing biogeochemical reaction networks and contributes key reactions where biogeochemical analyses are unequivocal. Our approach models the rate of nutrient uptake and the thermodynamics of coupled electron donors and acceptors for a range of microbial metabolisms, including heterotrophs and chemolitho(auto)trophs. Metabolism of exogenous substrates fuels catabolic and anabolic processes, with the proportion of energy used for each based upon dynamic intracellular and environmental conditions. In addition to biomass development, anabolism includes the production of key enzymes, such as nitrogenase for nitrogen fixation or exo-enzymes for the hydrolysis of extracellular polymers. This internal resource partitioning represents a trade-off against biomass formation and results in microbial population emergence across a fitness landscape. We use this model in initial simulations to explore the controls on community emergence and impact on rates of reactions that contribute to the cycling of carbon across distinct redox zones of an aquifer.

A Bioenergetic Approach to Constrain Substrate Quality in Carbon Turnover Models

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Decomposition processes dominate carbon cycling and feedbacks in terrestrial ecosystems by determining the rate at which assimilated C is returned to the atmosphere. Classical modeling approaches (Century, Daycent, RothC, CLM) treat decomposition as a first-order process: soil moisture and soil temperature are used to adjust a time-invariant decay rate that is specific to the "quality" of the substrate in a given C pool. In these models, microbial decomposition D_m in a specific C pool is calculated as

$$D_m = C_{stock}\boldsymbol{k}f_{moisture}f_{temperature}$$

with C_{stock} the amount of C in the pool decaying over time at a substrate specific rate k that is usually scaled by functions of moisture ($f_{moisture}$) and temperature ($f_{temperature}$). The C output resulting from decomposition is typically split into a flux R_H (heterotrophic respiration) that leaves as CO_2 and a fraction that is allocated to other C pools of lower "quality" and hence, slower decay rate $\boldsymbol{k}$.

This conceptual approach (= assign decay rates to given substrate categories and scale by moisture and temperature) has been successful in replicating observed C pools, but the ability of this modeling strategy to predict C pools in a changing environment is debated and is fundamentally restricted by the lack of meaningful molecular parameters to constrain the "quality" of the substrate.

Here, we present a new conceptual approach to the "quality" problem of decomposition. Our concept is based on the consideration that the intensity of decomposition processes should be correlated with the energy needs of the decomposer community. The energetic state of the substrate should thus be a major (if not the dominant) control on decomposition processes, together with considerations about microbial growth stage and resource supply (such as availability of terminal electron acceptors). Accordingly, a bioenergetic model describing the microbial processing of organic carbon is presented. Within this formulation, the fate of SOM is controlled by the average nominal oxidation state of its carbon, NOSC. This model posits that organic compounds whose NOSC ≈ 0 are more likely to be used to build biomass than more reduced or more oxidized organic molecules. That is, compounds such as acetate and glucose (NOSC = 0) are more likely to be used in anabolism than oxidized for energy (catabolism) to CO_2, because these compounds are near the average oxidation state of carbon of microorganisms. For instance, the average NOSC for the 20 regular protein-forming amino acids is +0.05. Converting carbon compounds with much higher or lower oxidation states into biomass would require more energy to process than those with a NOSC near 0. As a result, these relatively reduced and oxidized organic compounds should be preferentially used as electron donors in catabolic reactions. Finally, the rates of chemical reactions slow down as they approach equilibrium. Stated another way with regard to SOM, as the Gibbs energy, ΔG_r, of organic matter degradation gets closer to 0, the kinetics of this process also approaches zero. It follows that the oxidation state of carbon carries information about both the amount of energy stored *and* the rate at which this energy can be obtained. We posit that despite the fact that the structures and formulas, and therefore the thermodynamic properties, of the bulk of the compounds that comprise SOM are typically not known, the average nominal oxidation state of carbon, NOSC, can be used to estimate the energetic potential of SOM. Values of NOSC can be determined by the ratio of major elements (C, H, N, O, P, S) in organic matter.

Because the variables that determine Gibbs energies of reaction—temperature, pressure, and composition—are those that distinguish one soil environment from another, the approach described above should be applicable to any terrestrial setting and will allow us to compare the reactivities of organic compounds in different environments on the same parametric basis.

Reduced-Order Modeling of Fine-Resolution Hydrologic and Biogeochemical Simulations at NGEE-Arctic Study Sites

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As a major component of the hydrologic cycle, soil moisture plays a key role in a wide range of biological and biogeochemical processes. A high-resolution description of soil moisture is desirable for an improved investigation of regional-scale and watershed-scale phenomena. Direct deterministic simulations of fine-resolution land-surface variables including soil moisture present many challenges, a prominent one of which is the high computational cost. Previous work has focused on constructing fine-resolution solution fields based on statistical techniques. We instead propose the use of reduced-order modeling techniques to facilitate the straightforward emulation of fine-resolution simulations. We use an emulator, for example the Gaussian process regression, to approximate the fine-resolution 4D soil moisture fields. A dimension reduction technique known as "proper orthogonal decomposition" is further used to improve the efficiency of the resulting reduced order model (ROM). Apart from the initial computational overhead of constructing the ROM, subsequent use of the ROM has almost negligible computational cost. In addition, the ROM that we constructed is equipped with an uncertainty estimate, allowing modelers to construct a ROM consistent with uncertainty in the measured data. The ROM is also capable of constructing statistically equivalent analogues that can be used in uncertainty and sensitivity analyses.

We applied the technique to four polygonal tundra sites near Barrow, Alaska that are part of the Department of Energy's Next-Generation Ecosystem Experiments (NGEE)–Arctic project. Surface-subsurface isothermal flow simulations are performed for summer months using PFLOTRAN model for 100 [m] × 100 [m] domain centered on the four NGEE-Arctic study sites at 0.25 [m] horizontal resolution. The ROM is trained using simulated soil moisture from 1998–2000 and validated using the simulated soil moisture for 2002 and 2006. We present approaches to construct multiple types of ROMs for the NGEE-Arctic sites. Site-specific ROMs are capable of achieving pointwise relative accuracy that is >99%. Further, as generality of the constructed ROM increases (i.e., applicable to a wider range of sites), the more relevant statistical measures of error remain small. We also demonstrate the use of the ROM in several uncertainty quantification analyses and in understanding the impact of fine-resolution moisture heterogeneity on subsurface carbon dynamics and CO_2 emissions to the atmosphere.

Self-Organization, Emergence, and Fractal Dimension of Colloid Deposits in Model Soils

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Colloids, such as clay minerals, are ubiquitous in natural porous media. As a result, colloidal phenomena exert profound influence on subsurface hydrology, geochemistry, and microbiology. Certain common geochemical conditions generate colloid aggregation and colloid deposition, which are examples of self-organization at the colloidal scale that lead to emergent phenomena at larger scales. Here, we focus on the emergent property of permeability, the spatial distribution of which controls the magnitude and direction of fluid flow, and consequently the rate and extent of subsurface geochemical and microbiological processes. At a fundamental level, permeability is a function of pore-space geometry, which depends on colloidal phenomena. At least two mechanisms are relevant. First, colloid deposits reduce porosity, which reduces permeability as expressed, for example, in the Kozeny-Carman equation. Second, colloid deposit morphology has a major impact on permeability. This second mechanism has garnered less attention in the literature because of the difficulty in measuring colloid deposit morphology *in situ*. To address this gap, the research presented here used laboratory experiments to quantify deposit morphology with an innovative technique based on static light scattering (SLS) in refractive index matched (RIM) porous media. These experiments quantify two aspects of deposit morphology, fractal dimension and radius of gyration, both of which depend on hydrodynamic and geochemical effects (i.e., fluid velocity and ionic strength). For constant-flow experiments with constant influent colloid concentration and initially clean porous media, these experiments indicate that decreased permeability is associated with smaller fractal dimensions, that is, with colloid deposits having more dendritic and space-filling deposits. This result is consistent with previous research that quantified colloid deposit morphology using an empirical parameter. Modeling efforts are currently under way to correlate permeability with the underlying hydrodynamic and geochemical variables that control colloid deposit morphology. The relationship between permeability and colloid deposit morphology should also illuminate the more complex mechanisms of bioclogging, mineralization, and biomineralization. It is hoped that the insight gained will provide insight into other areas where porous media flow overlaps with colloid science: groundwater remediation, aquifer storage and recovery, petrology, and granular media filtration of potable water.

Complexity, Chaotic Dynamics, and Mathematical Modeling

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In many ways, complexity is just another name for multicomponent systems interacting in a nonlinear manner, and soil systems certainly fall within that category. Nonlinearity is the rule, because biological components (plants, microbes, etc.), which often represent the dependent variables of soil system models, are constantly changing the ways they interact, with some interactions being synergistic and others antagonistic. At each point in time, a given entity tries to optimize its individual condition, with the superposition of all this activity defining the state of the overall system. The question then arises, “What constitutes a healthy system?” When chaotic dynamics occur, the classical concept of ordered individual variation is lost, with time dependence becoming irregular, nonperiodic and unpredictable in the long term—hence the term “chaos.” However, we will argue that a new type of order appears at the system level in the form of an “attractor,” and this order needs to be better understood, because it represents the overall system. Another reason for current interest is that theoretical and experimental evidence has been accumulating that chaotic dynamics are probably ubiquitous in natural systems. In our opinion, three papers (Becks et al, 2005, *Nature Letters*; Graham et al. 2007, *Int. Soc Microb. Eco. J.*; Beninca et al., 2008, *Nature Letters*) have brought together, using experimental studies and relevant mathematics, breakthrough demonstrations that deterministic chaos is present in relatively simple biochemical systems (Molz and Faybishenko, 2013, *Procedia Environ. Sci.)*. These experiments are discussed, along with formulations and computer simulations of related models, including a mathematical model of rhizosphere dynamics (Kravchenko et al., 2004, *Microbiology*) driven by root exudation (Faybishenko and Molz, 2013, *Procedia Environ. Sci)*). Deterministic chaos may be viewed as a type of emergent phenomenon, and we present preliminary calculations suggesting that emergence is more likely to occur in systems with a spatial dependence as compared to fully mixed systems such as chemostats. We also suggest that nonlinear dynamics and deterministic chaotic processes may support the sustainability and resilience of ecosystems.

Mineral Interactions, Microbial Processes, and Transport Explain Long Residence Times of Rapidly Decomposable Deep Soil Organic Matter

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Using a new model (Biotic and Abiotic Model of SOM—BAMS1), we tested the hypothesis that observed long residence times of soil organic matter (SOM) are consistent with very labile organic compounds, nonequilibrium mineral interactions, microbial community dynamics, and vertical transport. BAMS1 is integrated in a three-dimensional, multiphase reactive transport solver and represents bacterial and fungal activity, archetypal polymer and monomer carbon substrate groups, aqueous chemistry, gaseous diffusion, aqueous advection and diffusion, and adsorption and desorption. The model results reasonably matched depth-resolved SOM and dissolved organic matter concentrations and fluxes in grassland ecosystems, and behaved consistently with expectations of depth-resolved profiles of lignin content and fungi:aerobic bacteria ratios. Microbial transformations of relatively labile organic compounds yielded predicted SOM turnover times consistent with observations and up to several thousands of years at depth because of transformation of plant material to microbial necromass protected on mineral surfaces and low concentrations of dissolved, assimilable substrate. While vertical transport was important in moving SOM below the zone of plant production, it did not explain the long residences times at depth. Thus, the persistence of intrinsically labile substrates and the increase in SOM turnover times with depth was caused by microbial activity, microbial transformation and necromass, and sorption kinetics. Finally, we discuss prospects for integrating this type of complex model structure into climate-scale models, like CLM, for prediction of global SOM dynamics under climate change.

The Kinematics of Root-Soil Interactions

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To understand spatial and temporal aspects of rhizosphere function, three points of view should be considered. From the point of view of the moving root tip, we see a chemical field surrounding the tip as the tip moves to deeper soil layers. A complementary perspective is the point of view of the stationary soil particle that will eventually lie beside a mature root cell. The fixed soil particle will experience the processes (efflux or uptake) associated with a neighboring root element, so that fluxes corresponding to the different root locations will be encountered in a predictable sequence. If the root tip is moving 0.5 mm h^{-1} downward, every half-hour the flux into or from the soil particle will be for a root element that is located 0.25 mm farther from the root tip. Thus, we can simplify the problem by imagining a stationary root, surrounded by a moving soil medium which is flowing 0.5 mm h^{-1} upward. Solving for the chemical field around the moving growth zone involves following a slice of soil as it moves upward, keeping track of the history of the radial profile and updating the chemical flux and diffusion over time as the soil encounters the older tissue elements. This approach is quite general and is illustrated for the computation of the pH in the soil around the tip of a growing root with known proton fluxes from the root surface. The third perspective is that of a particle attached to a cell initially on the surface of the root tip. This is the Lagrangian specification of root interaction with the soil. With time, the cellular particle accelerates away from the tip to reach a displacement velocity equal to the root elongation rate, as the cell decelerates to a final fixed location in the soil profile. Working simultaneously in the moving reference frame attached to the root tip and the stationary reference frame of the soil horizon is essential to understanding rhizosphere development and plant impacts on soil, yet few soil studies in the literature take root growth into account. The talk concludes with a summary of a new model for bacterial colonization of a growing root. The model by Dupuy and Silk shows that key traits for successful microbial colonization are root elongation rate, bacterial attachment rate and root cap carrying capacity.

A Zero-Sum-Game-Based Model for Litter Decomposition Dynamics

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Accurate representation of litter decomposition dynamics is a prerequisite for credible carbon-climate feedback predictions. However, most models rely on ad hoc parameterizations of lignin shielding, nitrogen stimulation, or nitrogen inhibition at different decomposition stages, and these parameterizations only agree with a subset of experiment data under specific environmental conditions. We contend that a more mechanistic treatment of carbon-nutrient interactions during decomposition could lead to more accurate and extensible model structures. We therefore propose and describe here a scalable zero-sum-game-based formulation of litter decomposition dynamics. We show that, because of binding site competition that occurs at different stages (e.g., limited microbial transporters, limited substrate surface area, and limited microbial metabolism capability), equilibrium chemistry kinetics and dynamic energy budget theory emerge as appropriate representations for decomposition dynamics. Our new model explains lignin dynamics and carbon-nitrogen interactions consistent with most litter decomposition experiments. Because our model formulation can resolve arbitrary levels of microbial community complexity and substrate diversity, we believe it will be a good prototype for modeling soil organic dynamics in earth system models and informing new empirical experiment design.

Thermodynamics and Pedogenesis Differences Between Desert Microsites

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Feedbacks exist between soil properties, climate, and ecological productivity. In arid alluvial fan deposits common to the southwestern United States, the strength of these complex feedbacks change slowly over long time frames (e.g., 10s to 100s of millennia) as the climate has become drier and warmer. The feedbacks are also influenced by relatively short-time-frame processes of shrub establishment and subshrub processes that create distinct interspace and subcanopy microsites. Pedogenic processes in both cases proceed at different rates—slowly in interspaces and rapidly beneath canopies—yet both are subject to similar energy and mass inputs entering the system from above the canopy.

In this study, we apply a branch of nonequilibrium (open system) thermodynamics to explain desert pedogenic processes and how the two microsites are tied together. The general concept is that energy and mass flow naturally in directions that minimize gradients, hence maximizing randomness and entropy. We hypothesize that younger soils begin as random bodies, but that energy input from the sun and mass input from water, dust, and vegetation create gradients over time, leading to microsites of pavements and canopies. These features eventually reach metastability, and the potential for self-destruction increases (i.e., desert pavements eventually fall apart and erode). We seek to apply these concepts to Mojave Desert soils/ecosystems that have been studied in the field and the laboratory, with the goal of explaining and/or predicting the pathways of pedogenesis in these environments. Of particular interest is how these concepts that might be applied in microsite locations influence the two-way coupling of pedologic development and ecosystem functions, and whether we can predict the strength of these feedbacks and processes using knowledge of soil systems today.

The field site is found in the Mojave Natural Preserve, CA, USA, where high spatial resolution infiltrometer measurements were taken along transects radiating from canopies of perennial shrubs into bare interspaces of structured soils. We augmented these measurements with ground-penetrating radar (GPR), laboratory analyses, and (in some cases) soil trenches. The results showed higher saturated conductivity under canopies versus interspaces, regardless of surface age, with the largest differences observed on older, developed soils. Bulk density, soil structure grade, and silt and clay content increased significantly away from the canopy, and organic content decreased toward interspaces. Trends in soil properties, from canopies to interspaces, were found to be predictable to a distance of 1.35 +/- 0.32 times the canopy radius, regardless of the size or genus of the shrub. The microsite environments, which are separated by only 10s of centimeters, release energy and mass at different rates—the fluxes differ by microsite locations. They exist with different thermodynamic gradients, with larger upward fluxes to support shrubs under canopy microsites, and larger downward fluxes in interspaces. Armor against change in interspaces can explain the progressive structural evolution of pedons, a paradoxically reduced water infiltration capacity, and a contraction of canopy volumes and ecosystem production in older soils. We use these gradients to illustrate the importance of microsite location when considering complex feedbacks that result through currently observed, time-dependent processes of pedogenesis in arid regions of the desert southwest.

Modeling Microbial Degradation of Soil Organic Matter with a Genome-scale Metabolic Reconstruction of Hopland Isolates

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Secreted plant exudates increase influx of labile C to soil, which impacts the dynamics of soil organic matter through changes in the activity of soil microorganisms. Presumably, uptake of plant exudates by microorganisms changes the C:N:P ratio within microbial cells. To maintain an optimal ratio, microbial cells activate certain metabolic pathways and produce extracellular products involved in degradation of the organic matter (e.g., glycoside hydrolases (GH), organic acids). However, the impact of plant exudates on microbial metabolisms still remains unknown, especially regarding which pathways are activated, and how exudates trigger secretion of extracellular enzymes.

Here we use genome-scale metabolic modeling and flux balance analysis, based on systemic stoichiometric, thermodynamic, and reaction capacity constraints, to simulate the metabolic fluxes and resulting phenotypes induced by different plant exudates. 37 Hopland isolates are used to choose the best candidate for the metabolic reconstruction. The main criteria are based on (1) selection of isolates with the highest genomic potential to produce glycoside hydrolases involved in the plant polymers degradation (GH1, GH3, GH5 CAZy families), (2) on the number of organic acid transporters encoded in the genome, (3) growth rate, and (4) abundance in the Hopland soil.

A draft model of the isolate is built from an annotated genome using the DOE Systems Biology Knowledgebase tools. Further manual reconstruction and refinement (gapfilling) is done by testing the growth of the isolate on C, N, P, and S sources using phenotypic microarrays (Biolog Inc.). Also, Biolog is used to confirm the ability of a microorganism to degrade plant polymers (pectin, mannan, dextrins, inulin, laminarin), and uptake *Avena sp*. exudates. We use metabolic footprinting to determine the exometabolome of the isolate, which includes uptake and secretion of compounds from/into the growth medium (plant exudates/extracellular enzymes). We further reconcile the metabolic model with experimental data to improve and validate its applicability.

This work will provide a genome-scale metabolic model that demonstrates how plant exudation impacts metabolic pathways of Hopland isolate, and triggers decomposition of organic matter through the production of extracellular enzymes. Furthermore, information on trade-offs between pathways obtained from the model will be used in Trait-based models at community scale.

Theme 4: Soil Systems and Global Climate Change

Bridging Soil Physics and Ecosystem Ecology towards Better Understanding Soil Trace Gas Efflux

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Trace gas emissions from soils are a measure of the metabolic activity by the community of microbes and roots in the rhizosphere. Knowledge of the connection between the physical and biological processes that drive these fluxes requires continuous flux measurements. We also need better soil efflux measurements to better partition net carbon fluxes into its constitutive components, canopy photosynthesis and ecosystem respiration. We have applied the eddy covariance (above and under plant stands) and arrays of flux-gradient systems to quantify fluxes on a quasi-continuous basis. In this talk, we describe some of the lessons learned based on our measurements over soils vegetated with oak savanna, annual grasslands, and deciduous and boreal forests.

Many models of soil respiration treat the soil as a dead black box, whose rates are modulated by temperature and soil moisture. These models must be highly parameterized. In practice, the magnitude and dynamics of soil trace gas effluxes are complex, and reflect the conditions of a living soil, or a live green box. Not only are these fluxes nonlinear responses to environmental variables like temperature and soil moisture, but they are often pulsed by rain and fluctuating water tables. The magnitude of the fluxes depends on phenology and the recent rates of photosynthesis. Moreover, the magnitude of the pulses depends upon antecedent conditions, which control the size of the more labile carbon pools, like the period of photodegradation and the number of prior rain pulses.

Predicting Soil Bacterial Responses to Multi-factor Global Change with Trait-based Modeling

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Soils harbor a tremendous diversity of microorganisms that influence ecosystem responses to environmental changes and feedbacks to climate. However, breaking down the soil microbial diversity into functional units and predicting their responses to multifactorial global changes remains intractable. Approaches that reduce community complexity to key functional traits are promising, but are still in their infancy for soil microorganisms.

Here, we coupled field measurements to a trait-based model to mechanistically evaluate the response of nitrite-oxidizing bacteria to a multifactorial global change field experiment in a California grassland. The experiment demonstrated that elevated CO_2, increased precipitation, and nitrogen addition, alone or in combination, altered the abundance, diversity, and activity of soil nitrite oxidizers that correspond to hundreds of phylogenetic units performing the second step of nitrification. However, the mechanisms explaining the observed global change effects were initially obscure. By characterizing and modeling three functional types of nitrite oxidizers spanning the trait-space of the NOB, we successfully captured the essential functional diversity within this bacterial group to further understand the observed responses to environmental change. In particular, the trait-based modeling approach resolved an emergent community structure consistent with the observations from different treatments, including the emergence of mixotrophic nitrite oxidizers (i.e. those able to use organic carbon in addition to oxidizing nitrite) under conditions of elevated CO_2, nitrogen, and precipitation. Inclusion of this functional type significantly improved the model predictions of the field nitrite-oxidation rate.

Our results are a starting point for representing the overwhelming diversity of soil bacteria by a few functional types that can be incorporated into terrestrial ecosystem models.

A Trait-based Model for Understanding Rates, Patterns, and Ecological Consequences of Microbial Nitrogen Fixation in High-Latitude Terrestrial Ecosystems

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Nitrogen limitation constrains primary productivity in high-latitude terrestrial ecosystems. In these ecosystems, biological soil crusts (BSCs) fix the vast majority of nitrogen, which becomes the dominant nitrogen source to the surrounding soil. Although it is pertinent to understand processes that control rates and patterns of nitrogen fixation in order to reduce uncertainties in the predictions of high-latitude soil carbon-climate feedbacks, few models take into account the environmental, ecological, and physiological constraints on nitrogen fixation. This work presents a model representing the spatial biogeography and activity of nitrogen-fixing and nonfixing microorganisms. We represent a number of functional guilds with different functional traits and capabilities associated with resource acquisition (e.g., carbon, nitrogen, phosphorus, and molybdenum) and environmental conditions (e.g., light, moisture, and temperature). The model resolves biogeographic areas that are dominated by N-fixers or non-N-fixers. The model also demonstrates that the rate of BSC nitrogen fixation is governed by seasonal factors (notably light and temperature), with higher rates of fixation during the growing season. However, we also note that heterotrophic nitrogen-fixers are active just prior to snowmelt, when cryptogamic crusts are inhibited by snow cover. An important aspect of the structure of the model is the inclusion of resource-acquisition investment that greatly constrains the biogeographical distribution of BSCs and impacts the rates and patterns of N fixation at the ecosystem level. Reducing the uncertainty associated with predictions of the fate of high-latitude soil carbon will require a mechanistic understanding of the nitrogen cycle under a changing climate. This model can significantly contribute to that goal.

The Pulsed Response of Soil Respiration to Precipitation in an African Savanna Ecosystem: A coupled Measurement and Modeling Approach

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Savannas cover 60% of the African continent and play an essential role in the global carbon cycle. The savannas of Africa are characterized by distinct wet and dry seasons, as well as a high degree of inter-annual variance in precipitation, which can produce pulsed inputs of moisture and subsequent pulsed responses of soil respiration to precipitation (hereafter called "pulsed responses"). Most studies on such pulsed responses have been conducted at the laboratory scale, and the importance of pulsed responses in the field setting is still not well understood. We proposed a modeling framework to describe the coupled dynamics of soil organic carbon (SOC), dissolved organic carbon, and microbial biomass in order to simulate pulsed responses. The developed model, along with high-resolution field observations of soil CO_2 concentrations, was then used to examine the importance of pulsed responses in an African savanna. Our results indicate that pulsed responses contribute to more than 20% of total soil respiration and more than 50% of soil heterotrophic respiration. Thus, pulsed responses are likely a key nonlinear and dynamic mechanism controlling soil carbon cycling in tropical savannas.

Hydromechanics of High-Elevation Meadows: Resiliency and Thresholds of Complex Soils

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While snowpack provides the dominant water-storage reservoir in mountain regions, the soil plays a fundamental role in secondary water storage and is a critical (and often overlooked) component of mountain hydrology. With their large quantity of stored carbon, high-elevation peatland soils provide essential ecosystem services related to water storage, filtration, and slow release to downstream communities—as well as carbon sequestration. Extreme dry years can cause the water table in these systems to drop below historic levels. This drying can induce changes in the structure of the soil through capillary consolidation, coupled to a simultaneous change in the decomposition rate of soil organic matter. Using a multiple method approach, we investigate the historic limit of dryness that high-elevation peatland soils in the Central Sierra Nevada have experienced in order to determine if future drying can trigger a hydrological tipping point resulting in an irreversible loss of ecosystem services. We found that within the historic limit of dryness (up to 0.04 bar suction), high-elevation peatlands are resilient and accumulating carbon. After exceeding the 0.04 bar dry limit, however, the peatlands begin to consolidate, leading to loss of porosity and permeability, and loss of soil carbon through decomposition. In addition, we show that the structural changes in the soil are rapid, have immediate consequences for high-elevation peatland resilience, and have a disproportionately large impact on hydrology in comparison to decomposition. This research highlights how small changes in climate can trigger local hydrologic tipping points in mountainous regions, with cascading regional-scale impacts.

The Microbial Ecology of Soil Carbon

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The identities of organisms profoundly influence ecosystems, and microbial diversity is vast. Yet, the hackneyed “black box” of microbial ecology persists: we ecosystem scientists ignore and collapse microbial diversity into a box and a few arrows. We do this because this has been and still is a useful approach on scales relevant for biogeochemistry. Insights from molecular tools to the microbial world do not yet connect strongly to quantitative biogeochemistry. Yet there is good reason to try to make this connection, and there are promising new approaches for doing so. Here, I will frame this problem in the context of the quantitative microbial ecology of soil carbon.

Permafrost Carbon-Climate Feedback: Sensitivity to Deep Soil Decomposability and Nitrogen Cycle

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Permafrost soils represent a significant potential carbon-climate feedback, through enhanced decomposition accompanying thaw. In addition to releasing greenhouse gases, enhanced decomposition may increase N mineralization as well, leading to increased plant growth and a negative carbon-climate feedback. Furthermore, the dynamics of deep carbon may differ from that of shallow soils, and thus there remains a large uncertainty regarding the fate of buried soil organic matter after thaw. We examine the sensitivity of a carbon-nitrogen model that includes permafrost processes, CLM4.5-BGC, to these multiple effects under a set of offline transient warming experiments over the period 1850-2300, and calculate feedback parameters for the permafrost region based on these model integrations. Our results suggest that nitrogen responses, while present, are insufficient to offset projected carbon losses when deeper SOM is allowed to decompose upon thaw, with total carbon losses from the region of 21-164 Pg C, depending on parameter values chosen.

Non-linear Response of Soil Carbon Gas (CO_2, CH_4) Flux to Oxygen Availability

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Soil oxygen (O_2) concentration can impact soil-atmosphere fluxes of carbon dioxide (CO_2) and methane (CH_4), and contribute large differences in soil carbon (C) storage at local to landscape scales. Soil O_2 is increasingly being measured to explore redox dynamics even in drained upland soils, but few studies have established quantitative relationships between gas-phase O_2 concentration and soil C fluxes in controlled settings. Though various intrinsic biological (Michaelis-Menten enzyme kinetics) and extrinsic physical (gas or substrate transport) mechanisms could lead to highly nonlinear relationships between O_2 concentration and C gas fluxes, existing laboratory studies have imposed coarse or narrow changes in O_2 concentration that necessarily prevent detection of nonlinearity. We report on the results of laboratory incubations designed to explore the short-term sensitivity of soil CO_2 and CH_4 emissions to a wide range of gas-phase O_2 concentrations. An organic-rich Histosol was collected from a drained peatland and subjected to seven O_2 concentration treatments ranging from 0.03% to 20% O_2. We compared the fit of the observed C flux response to O_2 concentration to linear and nonlinear (log) model, and used the coefficient of determination (R^2) and distribution of residuals as model performance metrics.

Soil CO_2 fluxes increased ($P < 0.001$) with increasing O_2 concentration from 180 ± 5 μg C g^{-1} d^{-1} at 0.03% O_2 to 227 ± 16 μg C g^{-1} d^{-1} at 20% O_2 whereas soil CH_4 fluxes decreased ($P < 0.001$) from 303 ± 32 ng C g^{-1} d^{-1} to 77 ± 11 ng C g^{-1} d^{-1} across the same range of O_2 concentrations. Net CH_4 emission rates were attenuated at higher O_2 concentrations, most likely owing to stimulation of gross CH_4 consumption. A log-linear fit outperformed a linear model fit for gas-flux response to O_2 concentration: log-linear R^2 values were 0.49 and 0.70 for CO_2 and CH_4 flux respectively, in contrast to 0.38 and 0.40 for the linear model. This study demonstrates the importance of O_2 in regulating soil C gas emissions and supports significant effects of even *trace* concentrations of O_2 in soils.

**Biogeochemistry of the Microbial Soil Sink of Carbonyl Sulfide (COS)—
A Carbon-Cycle Tracer**

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Soils microorganisms access their repertoire of genetic tools for survival in response to the availability of substrates from the organic, mineral, aqueous, and gaseous phases present in their microenvironment. Their collective metabolism has a profound effect on the cycling of elements within soils and the exchange of gases between the atmosphere and soils. One such example is the cycling of carbonyl sulfide (COS), a trace constituent of Earth's atmosphere (global mean of ~500 pmol mol^{-1}), which has a significant global soil sink thought to be driven by microorganisms containing carbonic anhydrase (CA) enzymes that catalyze the hydrolysis reactions of both COS and carbon dioxide (CO_2): $COS + H_2O \rightarrow CO_2 + H_2S$ and $CO_2 + H_2O \rightleftharpoons HCO_3^- + H^+$. Because of this shared reaction of COS and CO_2 via CA in plants, measurements of COS hold great promise as a tool for disentangling the large, simultaneous photosynthetic and ecosystem respiration CO_2 fluxes of the terrestrial biosphere, which is critical for assessing changes in carbon sequestration in response to climate forcing. Cautious application of COS as a carbon-cycle tracer requires that other ecosystem fluxes, such as COS soil uptake, be understood well enough to be accounted for.

In this project, we are interested in linking gene-, microbe-, and mesoscale processes regarding soil cycling of COS with the hope of identifying the key processes influencing macroscopic soil-atmosphere fluxes of COS. We use gene-based discovery to link soil microorganisms, their CA enzymes, and COS consumption. In particular, we aim to link atmospheric COS uptake to the specific type and clade of CA, and use bioinformatics to determine the breadth of distribution across common soil phyla. Furthermore, we seek to shed light on whether microorganisms consume COS as part of a sulfur assimilation pathway, as is the case for plants, or if COS is simply hydrolyzed by CA due to a structural similarity of COS and CO_2. Advances made in understanding the use of COS at multiple scales in complex soil environments will help inform understanding of soil sulfur cycling, and are imperative for the process-level understanding and prediction of soil-atmosphere exchange of COS.

Mesoscale Soil-Surface Heterogeneity as a Controlling Influence on the Generation of Macropore Flow

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The key concept in the initiation of macropore flow at the land surface is that water is applied faster than it can infiltrate into the soil matrix material. Sometimes this condition is associated with matrix saturation and ponding, but accumulated evidence shows that preferential flow is commonplace in soils whose moisture states are substantially less than saturated and whose macropores are not completely filled. Examples include macropore infiltration into shrinkage cracks of dry soil, locally focused water that enters a macropore when it fails to infiltrate in hydrophobic matrix material, and free-surface film flow generated by conditions of matrix-to-macropore seepage. A more widely applicable generalization is to consider localized overland flow generated on a small area of relatively impermeable soil associated with a macropore. Water that collects on such an area could initiate preferential flow on a mesoscale basis when water currently available at the land surface exceeds the infiltration capacity of that area. Thus, a useful model can be based on the distribution of patches of low-infiltrability soil surface.

This new model considers two levels of important elementary areas. One is the traditionally employed representative elementary area (REA), which includes an adequate variety of small-scale heterogeneities to typify larger areas within the same field. This is the area appropriate to determination of infiltration capacity of a plot or field by standard definitions and methods. The other is a localized area smaller than the REA, and large enough to include numerous pore-scale features, but not including enough heterogeneities to represent an area larger than itself. This smaller area, here called a functional sub-area (FSA), constitutes a functional unit that can be represented by a single value of localized infiltration capacity. The REA is considered as a mosaic of FSAs.

When water is applied to the land surface by rain, irrigation, or other means, each FSA absorbs water into its soil matrix material up to the rate of its localized matrix infiltration capacity. Any water applied in excess of that rate is assumed to flow into a macropore within or adjacent to the FSA, thus becoming preferential flow. Especially if crusted or hydrophobic, an FSA can generate significant preferential flow even during low-intensity rainfall when most other FSAs are absorbing all incident water into the matrix. The soil surface is not represented by a single value of infiltration capacity, but rather by a characteristic distribution of values. The total flux of preferential flow at a given depth, considered at the REA scale so that its measurement represents the behavior of the soil as a whole, is the sum of the contributions from all FSAs. In this way, the mesoscale heterogeneity controls the field-scale partitioning of matrix and macropore flow as an emergent phenomenon.

Illustrative case studies from diverse agricultural sites use field-measured data including water application rate, soil water conditions, and preferential flow evaluated from tile drainage or water table fluctuations. Tests show that this model can explain and quantitatively represent observations of preferential flow occurring in relatively dry soils or at modest rainfall intensities. The results indicate that properties and mesoscale heterogeneity of soil matrix material, independent of preferential flow-path characteristics, can be a controlling influence on the generation of macropore flow.

Classifying the Visual Quality Assessment of Time Series Data into Data Quality Patterns

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Soil-systems research makes extensive use of observational data, in particular data collected by sensor systems and data used for integrated perspectives on biogeophysical systems. One of the main components of using observational data is quality control. Observational data are subject to many sources of problems, ranging from sensor malfunctions to post-processing data formatting mistakes. Quality assurance activities are therefore essential to allow use of observational data with any degree of confidence. Identification of error patterns can provide critical information needed for the uncertainty quantification of complex phenomena. To make reliable predictions of complex climatic phenomena, it is important to distinguish real process uncertainty from data problems. While some quality assurance methods can be automated, most of them are often heavily dependent on the domain and with previously unknown types of problems frequently appearing, automation efforts are challenging.

In this work, we explore methods to identify and classify data problems, better characterizing them for subsequent implementation of automated detection methods. This identification step allows for creation of quality control tools that are more general and, more importantly, tools that can be systematically evaluated. The main data set we used in this work includes carbon, water, and energy fluxes data collected alongside micro-meteorological and biological variables across field sites that are part of FLUXNET. These data not only include monitoring of several variables relevant to soil systems, but many of the issues identified are relevant for long-term monitoring efforts.

We present here the patterns identified, as well as common causes for the issues they cover and possible strategies for correction.

The Role of Hydrodynamic Methane Transport in Soil-Atmosphere Methane Fluxes in a Temperate Marsh

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Soil-atmosphere fluxes of methane occur via several transport processes in wetlands. While the importance of ebullition (bubbling) and the plant-mediated transport are widely acknowledged, transport of dissolved methane through the surface water is commonly perceived to be negligible. Recent observations and laboratory experiments hint that this methane transport can be important under certain meteorological conditions. We evaluated the contribution of the hydrodynamic transport of dissolved methane over a year at a temperate marsh. We quantified dissolved methane transport across the air-water interface using a modeled gas transfer velocity and biweekly measurements of dissolved methane concentration in the water column. We then compared this methane transport to net soil-atmosphere methane fluxes measured via eddy covariance. Over the yearlong study period, we found the contribution of dissolved methane air-water transport to net soil-atmosphere methane fluxes to be surprisingly large. Thermal convection occurring overnight as the marsh water surface cooled spurred hydrodynamic dissolved methane transport that accounted for more than half of all nighttime methane fluxes. Overall, transport of dissolved methane through the surface water was responsible for 30% of annual methane fluxes. These findings indicate that for wetlands with a water table above the ground surface, a significant portion of methane fluxes to the atmosphere may be neither plant-mediated nor due to ebullition. Including methane transport through surface water driven by surface cooling or other meteorological forcing in methane models may improve predictions of both the timing and magnitude of soil-atmosphere methane fluxes.

Climate Change Effects on Inorganic and Organic Carbon Cycling in Soils

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Climate change will significantly affect soil properties and fertility, water resources, food quantity and quality, and environmental quality. The soil C pool includes both inorganic C (IC) and organic C (OC) (living organisms and organic compounds). On a global scale, more than 75,000,000 Gt of C is present within the global C lithospheric pool; by far, the largest quantity of C, more than 60,000,000 Gt, is in the form of sedimentary carbonates. Other C pools include 720 Gt in the atmosphere and 38,400 Gt in the oceans. While much of the lithospheric C may currently be unavailable to C cycling, abiotic processes associated with climate-induced soil acidification and accelerated mineral weathering could redistribute large quantities of C among the Earth's three major C pools (land, atmosphere, and oceans).

Soils play a large role in global cycling of IC and OC. About 2500 Gt C is stored in soils, of which 1550 Gt are OC and 950 Gt are IC. Further, a substantial amount of the IC pool is present in the form of carbonates, such as calcite. Abiotic C cycling and its influence on the IC pool in soils is a fundamental global process, in which acidic atmospheric CO_2 participates in the weathering of carbonate and silicate minerals, ultimately delivering bicarbonate and Ca^{2+}, or other cations, that precipitate in the form of carbonates in soils or are transported to the rivers, lakes, and oceans. In addition, biotic processes consume atmospheric CO_2 and create organic carbon (C) that is either reprocessed to CO_2 or stored in soils. Clearly, soil response to climate change will be complex, and the impacts of many climate change variables on relevant reactions, processes, and the soil sink/source behavior remain largely unknown. The objective of this presentation is to initiate and further stimulate a discussion about some important and challenging aspects of climate-change effects on soils, such as accelerated weathering of soil minerals and resulting C and elemental fluxes in and out of soils, soil/geo-engineering methods used to increase C sequestration in soils, soil organic matter (SOM) protection, transformation and mineralization, and SOM temperature sensitivity. This presentation includes recent discoveries and identifies key research needs required to understand the effects of climate change on soils.

Assessing Kinetics of Fe Reduction and Degradation of Organic Matter in Subalpine Wetland Soils

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The biogeochemical cycles of iron (Fe) and carbon (C) are closely linked due to the interactions between Fe mineral phases and organic matter. The Fe cycle is controlled partly by the shifts in redox conditions, leading to either mineralization of Fe(III) or mobilization of Fe(II). In soils, Fe(III) gets reduced abiotically and to a significant extent microbially. Various microorganisms can use Fe(III) as a terminal electron acceptor for respiration coupled to the oxidation of C. Wetlands are unique environments because of their organic-rich hydric soils, which act as a carbon sink and retain inorganic and organic contaminants. However, climate change accompanied by a potential temperature rise in subalpine wetlands could enhance the decomposition of organic matter and therefore increase the microbial Fe fluxes in soils. As an aftermath of an accelerated Fe flux in wetlands, the release of contaminants would potentially increase, and carbon sequestration would be diminished. Therefore, investigators must quantify the key kinetics of biotic Fe reduction to understand and predict the biochemical fate and transport of organic C and contaminants in wetlands.

We studied the kinetics of microbial Fe(III) reduction in soils of three hydrogeomorphically different wetlands with seasonally varying or constant redox potentials. The wetlands are located in a subalpine conifer forest at elevated altitude (2700–3300 m) and are part of the USDA Fraser Experimental Forest, Colorado (USA). We performed flow-through reactor (FTR) experiments to investigate Fe reduction rate and carbon release rate from dissolved organic matter. The flow-through reactors consist of intact soil cores (2 cm L, 4.7 cm ID) sampled at two different depths (20-30 and 50-60 cm) preserved under anaerobic conditions. In our ongoing experiments, the natural Fe-reducing microbial consortia are stimulated by introducing synthetic pore-water solution along with varying concentrations of Fe(III) as Fe-NTA (0.1 to 2.5 mM) at three different temperatures (6°, 12°. and 18°C) encountering the temperature range at the subalpine field site. Fe(III)-NTA is considered a biodegradable model compound for iron complexes present in natural organic matter. To monitor Fe(III) reduction and carbon degradation from organic matter, we measured total Fe, dissolved Fe(II), and dissolved organic carbon in the FTR effluent.

For all tested soil cores, our preliminary results showed a fast Fe(III) breakthrough with Fe(III) outflow concentrations that initially increase before reaching a plateau. This steady state was reached within 0.5 to 2.5 days after changing temperature or concentration of the input solution. A comparison of Fe(III) in the inflow and outflow indicates 44% to 92% Fe(III) reduction in all three wetland soils, with negligible difference for the two depths investigated. With higher reduction of Fe(III)-NTA, we also observed an increase in the release of organic C as dissolved organic carbon.

This ongoing experimental work will determine the kinetics of Fe reduction and dissolved organic carbon transformation. Further work will also characterize the distribution of Fe-reducing bacteria and Fe mineralogy of the intact soil cores before and after the FTR-experiments.

Physical and Biological Processes Interact To Determine Soil Carbonyl Sulfide Uptake in Two Contrasting Ecosystems

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Carbonyl sulfide (COS) is a promising tracer for studies of carbon cycle processes at regional to continental scales. This requires knowledge of soil COS fluxes, considered the second largest COS sink after vegetation at the global scale. Similar to leaves, COS uptake in the soil is catalyzed by the enzyme carbonic anhydrase active in soil microorganisms. Estimates of soil COS fluxes have been limited by the lack of field observations. We report field data on soil COS and CO_2 fluxes from two sites with contrasting soil conditions: a dry oak woodland in southern California, and a wet tropical rainforest in Costa Rica. We measured soil COS and CO_2 fluxes in dynamic chambers coupled to a laser spectrometer. At both sites, we measured litter COS fluxes separately from surface (soil+litter) fluxes. Soil and litter were primarily COS sinks. Although water status was a main driver of COS uptake at both sites, we noted important differences. At the dry site, the soil was covered with a thick litter layer that contributed up to ~90% to surface COS uptake, particularly after rewetting events. Concurrent bursts of respiration and COS uptake after rewetting indicated that the soil and litter microbial activity were strongly water limited. In contrast, COS uptake decreased with soil water content at the wet site, indicating diffusional limitation to uptake when soil pores become water filled. At the rainforest site, we also characterized the soil microbial community. Along a short transect, the microbial community structure followed the same gradient as the soil moisture, but was not correlated with soil COS uptake. Thus, the physical soil status may be more important than the microbial community structure in determining soil COS uptake when soil moisture is not limiting. We constructed a diffusion-reaction model with data-driven optimization of COS uptake and production activity parameters in the soil and litter. The simulated fluxes agree well with field observations at both sites. Our results indicate that surface COS fluxes in dry ecosystems may have a more pronounced and opposite seasonality to fluxes in wet ecosystems. The seasonality of litter input and speed of litter decomposition are therefore useful parameters to consider in long-term or large-scale simulations of surface COS fluxes.

Resolving Terrestrial Ecosystem Processes along a Subgrid Topographic Gradient for an Earth-System Model

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Soil moisture is a crucial control on surface water and energy fluxes, vegetation, and soil carbon cycling. Earth System Models (ESMs) generally represent an areal-average soil-moisture state in gridcells at scales of 50 to 200 km, and as a result are not able to capture the nonlinear effects of topographically controlled subgrid heterogeneity in soil moisture—in particular where wetlands are present. We addressed this deficiency by building a subgrid representation of hillslope-scale topographic gradients, TiHy (Tiled-hillslope Hydrology), into the Geophysical Fluid Dynamics Laboratory (GFDL) land model (LM3). LM3-TiHy models one or more representative hillslope geometries for each gridcell by discretizing them into land-model tiles hydrologically coupled along an upland-to-lowland gradient. Each tile has its own surface fluxes, vegetation, and vertically resolved state variables for soil physics and biogeochemistry. LM3-TiHy simulates a gradient in soil moisture and water-table depth between uplands and lowlands in each gridcell. Three hillslope hydrological regimes appear in nonpermafrost regions in the model: wet and poorly drained, wet and well drained, and dry; with large, small, and zero wetland area predicted, respectively. Compared to the untiled LM3 in stand-alone experiments, LM3-TiHy simulates similar surface energy and water fluxes in the gridcell-mean. However, in marginally wet regions around the globe, LM3-TiHy simulates shallow groundwater in lowlands, leading to higher evapotranspiration, lower surface temperature, and higher leaf area compared to uplands in the same gridcells. Moreover, more than four-fold larger soil carbon concentrations are simulated globally in lowlands as compared with uplands. We compared water-table depths to those simulated by a recent global model-observational synthesis, and we compared wetland and inundated areas diagnosed from the model to observational datasets. The comparisons demonstrate that LM3-TiHy has the capability to represent some of the controls of these hydrological variables, but also that improvement in parameterization and input datasets are needed for more realistic simulations. We found large sensitivity in model-diagnosed wetland and inundated area to the depth of conductive soil and the parameterization of macroporosity. With improved parameterization and inclusion of peatland biogeochemical processes, the model could provide a new approach to investigating the vulnerability of boreal peatland carbon to climate change in ESMs.

Microbial Ecology across Polygon Types and Features at the NGEE-Arctic Barrow Site

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Arctic soils contain an estimated 12–42% of terrestrial carbon, most of which is sequestered in permafrost. High latitudes have experienced the greatest regional warming in recent decades, and observations suggest that permafrost degradation is now commonly observed in the region. With increasing global temperatures, permafrost soils are becoming a potential source of greenhouse gas (GHG) emissions. Because of widespread permafrost thaw, much of the soil organic matter may be available for rapid mineralization by microorganisms in the soil. Yet little is known about the vulnerability of permafrost and the potential response of soil microorganisms to availability of new carbon sources. On the Alaskan North Slope, the collapse and rise of soil due to formation of ice wedges and permafrost thaw create distinct features called polygons. As part of the U.S. Department of Energy (DOE) Next Generation Ecosystem Experiment (NGEE) in the Arctic, we aimed to determine the distribution of microbial populations across a range of polygon features and to correlate the microbial data to GHG flux data. To determine the microbial community distribution and metabolic potential, we collected seasonally thawed active layer soil samples along two polygon transects (Site 0 and AB), including high-centered, transitional and low-centered polygons. Illumina HiSeq technology was used to sequence 16SrRNA genes and metagenomes from these active layer soils. The sequence data was correlated to GHG flux measurements and to environmental data from the site, including geophysical and geochemical soil characteristics. Both the microbial communities and the flux measurements varied along the polygon transect. Each polygon type had a distinct microbial community structure; however, these microbial communities shared many metabolic capabilities. For example, many genes involved in degradation of chitin could be found all three types of polygons. Functional genes involved in methanogenesis and CH_4-flux measurements were higher in low centered and wetter polygons than in high centered and drier polygons. Within all polygon regions, the microbial community composition and flux data were indicative of CO_2 production. The metagenome sequence data suggested that nitrate was utilized as a nitrogen source, but not lost through denitrification. The long-term goal is to use information gleaned from omics datasets to better inform climate models.

The Effect of a Warmer Climate on Soil Carbon Cycling: Emergent Responses across Time and Space Scales

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Globally, atmospheric warming is the most certain climate impact of increasing atmospheric greenhouse gas concentrations. This warming will lead to warmer soils fairly rapidly. For example, 80% of a step-change in air temperature will be realized at 1 m depth within a year (all else equal). It is well established that temperature has immediate, direct effects on decomposition rates (e.g., through effects on enzyme activity, binding energies, and reaction kinetics). At longer time scales, evidence is emerging for microbial acclimation or changes in carbon use efficiency. Perhaps even more challenging, longer time scales of warming will lead to changes in vegetation, soil properties, and even, in permafrost regions, large changes in landscape topography and inundation. These ecosystem- and landscape-level impacts of warming may dominate the effects of climate change decomposition and soil carbon losses, and need to be integrated into our experimental and predictive frameworks.

Capturing Transient Climate-Driven Contributions of Surface-to-Subsurface Processes at Watershed Scales

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The response of humid mid-latitude forests to changes in precipitation, temperature, nutrient cycling, and disturbance is critical to improving our predictive understanding of ecosystem-climate feedbacks to greenhouse gas fluxes and changes in the surface-subsurface energy balance. Predictive understanding of terrestrial systems will require an integrated modeling/experimental approach applied across multiple scales. Recent scientific advances in computing, spectroscopy, and "-omics" enable unprecedented process-level studies to address critical knowledge gaps. Mechanistic understanding of the effects of long-term and transient moisture conditions are needed to quantify linkages between changing redox conditions, microbial activity, and soil mineral and nutrient interactions on C cycling and greenhouse gas release in surface-to-subsurface transition zones.

The objective of this effort is to improve mechanistic understanding of the of long-term and transient soil moisture dynamics on C cycling in surface-to-subsurface transition zones. Specifically, we hypothesized that variations in soil moisture govern complex biogeochemical responses affecting the C processing and greenhouse gas production.

To study these concepts, we established transects across hydraulic and topographic gradients in a small watershed with transient moisture conditions. Valley bottoms tend to be more frequently saturated than ridge tops and side slopes, which generally are only saturated when shallow storm flow zones are active. Fifty shallow (~36") soil cores were collected during time frames representative of low CO_2, soil winter conditions and high CO_2, soil summer conditions. Cores were subdivided into 240 samples based on pedology and analyses of the geochemical (moisture content, metals, pH, Fe species, N, C, CEC, AEC) and microbial (16S rRNA gene amplification with Illumina MiSeq sequencing) characteristics are being conducted. To associate microbial metabolic activity with greenhouse gas emissions, we installed 17 soil gas probes, collected gas samples for 16 months, and analyzed them for CO_2 and other fixed and greenhouse gases. Surface water and groundwater data are also available.

Parallel to the experimental efforts, our data is being used to support hydrobiogeochemical process modeling by coupling CLM with PFLOTRAN to simulate processes and interactions from the molecular-to-watershed scales. Including aboveground processes (biogeophysics, hydrology, and vegetation dynamics), CLM provides mechanistic water, energy, and organic matter inputs to the surface/subsurface models, in which coupled biogeochemical reaction networks are used to improve the representation of belowground processes. Preliminary results suggest that inclusion of aboveground processes from CLM greatly improves the prediction of moisture response and water cycle at the watershed scale. We are investigating the coupled biogeochemical C, N, P, and Fe cycles in the surface and subsurface with improved biogeochemical models that incorporate geochemical and microbial reactions for process-based representation. The results will improve our understanding of the coupled hydrobiogeochemical processes at multiple scales and the representation of these processes in earth system models.

Microbes as the Living Component of Complex Soil Systems: Data and Models

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As living components of complex soil systems, soil microbes play a fundamental role in nutrient biogeochemical cycling and trace gas fluxes, which affect the behavior of the climate system. Eventually, except for a few minor physical and chemical processes, soil microbes are the only avenue for the decomposition of soil organic carbon and its release to the atmosphere. Therefore, it is critically important to investigate soil microbes and their roles in nutrient cycling and trace gas production and consumption within complex soil systems, in order to address global change problems. However, there are large gaps in this direction, mostly due to the difficulties involved in *in situ* monitoring of single microbial processes, and the lack of understanding with respect to some critical microbial processes in complex soil systems. (For example, the microbial species involved in methane production are still far from certain, although the genes for this function could be easily pinpointed and a group of Achaea has been identified as primary methanogens.) Furthermore, most extant ecosystem-level models ignore microbes or simply treat them as one active carbon pool, and the real mechanisms for microbial regulation of nutrient cycling and microbial contribution to landscape trace gas flux in the complex soil systems are implicitly considered in the models.

We began our research effort from a modeling perspective, targeting the question of how soil microbes contribute and respond to climate change by using a data-model integration approach. Approximately 3458 data points for soil microbial biomass carbon (C), nitrogen (N), phosphorus (P), and/or sulfur (S), and 2630 data points for soil microbial turnover were compiled. Then, we estimated the soil microbial biomass carbon, nitrogen, and phosphorus, and their stoichiometry across the globe, as well as the mean residence time of soil microbes in soils. We estimated that soils contain 16.7 Pg C (1 Pg = 10^{15} g) and 2.6 Pg N in 0–30 cm soil profiles, and 23.2 Pg C and 3.7 Pg N in 0–100 cm soil profiles. The best estimate of *C:N:P* stoichiometry is 41:6:1 for soil microbial biomass, compared with 287:17:1 for soil organic matter. After adjusting for the temperature difference between incubation experiment and annual average, mean residence time of the microbial biomass carbon in the soil was ~23 days, with a 90% confidence interval of 1–200 days, which is inconsistent with the estimated modeled mean residence time for microbial biomass carbon based on soil heterotrophic respiration. Meanwhile, there are substantial spatial heterogeneities in the soil microbial biomass and its turnover rate. These field estimates were compared against the results of earth system models used for IPCC reports; there are large discrepancies in terms of microbial contribution to the heterotrophic respiration. The high-latitude regions are greatly underestimated in their microbial contribution to carbon cycling. The knowledge obtained through this study provides fundamental information for untangling complex soil systems and how they biologically work.

Theme 5: Using a Complex System Approach for Practical Applications

Latent Approaches to Linking "Omics" with Belowground Processes: A Methane Case Study

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The increasingly widespread use of microbial "omics" has the potential to answer unresolved questions and generate novel hypotheses about belowground ecosystem processes, such as methane cycling. However, one key challenge involves relating small-scale data concerning functional gene "blueprints" and activity to soil processes assessed at the plot level and beyond. At higher scales, microbial populations and activities are not measured directly; a classic case of latent variables. We present a latent framework to analyze ecosystem processes empirically with functional gene data via structural equation modeling, using methane cycling as a case study.

At field sites on Vancouver Island, B.C., we investigated the impact of environmental factors and functional gene abundances on CH_4 surface emissions along a moisture and forest type gradient over a growing season. Gene abundances for methane-related genes (microsite scale) were assessed at 10 and 20 cm. Methane surface exchange and belowground concentrations at 10 and 20 cm were measured. We created an exploratory conceptual model to link microsite gene expression data with plot-level CH_4 surface exchange, and environmental data. Using structural equation modeling, we grouped together gene abundances (pmo, mcr ,amo and variants) as a plot-level latent variable to determine its effect on CH_4 surface exchange relative to environmental factors, as well as effects of environment on gene abundances. We found that grouping gene abundances into a latent variable was able to account for approximately 26% of the variation in surface CH_4 emissions.

Our results lay the conceptual groundwork to construct a more complex model incorporating more genomic data (e.g., transcriptome data) as well as increased temporal and spatial coverage of all the observed variables. We will also discuss issues and possibilities using structural equation modeling in conjunction with ordination and hierarchical spatial models to generate basic knowledge and contribute to better management of soil ecosystems. Finally, we will also present conceptual models to apply this approach to N_2O emissions and the role fungal symbioses in carbon cycling.

Willow Growth and Bioaccumulation of Contaminant Metals: Links with Dominant Ectomycorrhizal Fungi

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Willows are fast-growing plants that perform well under harsh conditions, and are potential candidates for the removal of excess metals from contaminated soils. In practice, the success of phytoremediation has varied, but our inability to reliably predict remediation outcomes may be related to our limited understanding of how plants interact with microbial communities in contaminated soils. We previously observed strong selection for ectomycorrhizal fungi, notably *Sphaerosporella*, in the rhizosphere of certain willow species in hydrocarbon-contaminated soils. The absence of this selection pattern in uncontaminated soils showed that the presence of contaminants can completely alter plant-microbe associations.

In this study, we planted three willow species in a block design across a metal contamination gradient at the site of a former military landfill. Our aim was to determine whether certain rhizosphere microbes were associated with efficient metal sequestration by plants. Using the high-throughput Ion Torrent sequencing platform, we sequenced bacterial (16S rRNA gene) and fungal (ITS) communities from bulk soil 2 weeks after planting, and at 4 and 16 months post-planting from the rhizosphere of destructively harvested willows. We also quantified willow biomass, total and water-soluble concentrations of 6 metal contaminants (As, Cd, Cu, Ni, Pb, and Zn) in the soil, total concentrations and tissue allocation of the same metals within willows, and a range of additional soil parameters. After 4 months, most willow rhizosphere soils were dominated (50-90% of relative sequence abundance) by one of three ectomycorrhizal fungal taxa: *Sphaerosporella*, *Geopora*, or *Inocybe*. The abundance of these three primary colonists had decreased dramatically 16 months after planting, accompanied by a large increase in total fungal diversity. Interestingly, willows with dominant *Sphaerosporella* and *Inocybe* populations after 4 months showed higher Zn bioaccumulation in shoots, while willows with dominant *Sphaerosporella* populations also demonstrated a higher average total biomass.

Overall, *Sphaerosporella* was the taxon most strongly associated with total Zn uptake by willows, which was most successfully phytoextracted metal at the site by a large margin. When *Sphaerosporella* and *Inocybe* were the dominant rhizosphere fungi, total fungal diversity was strongly and negatively related to willow Zn bioaccumulation, suggesting that competition between rhizosphere colonists may limit phytoremediation activity. Although controlled experiments are required to confirm the direct role of these ectomycorrhizal fungi in facilitating metal uptake by willows, these data suggest that the formation of appropriate plant-microbe relationships may be a critical component of phytoremediation success.

Increased Crop Yields and Differing Soil Properties as a Result of Two Native Woody Shrubs in the Peanut Basin, Senegal

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A changing climate, along with human and animal population pressure, can have a devastating effect on crop yields and food security in the Sudano-Sahel. Agricultural solutions to address soil degradation and crop-water stress are needed to combat this increasingly difficult situation. Significant differences in crop success have been observed in peanut and millet grown in association with two native evergreen shrubs, *Piliostigma reticulatum*, and *Guiera senegalensis*, at the sites of Nioro du Rip and Keur Matar, respectively. In this study we investigate how farmers can increase crop productivity by capitalizing on the evolutionary adaptation of native shrubs to the harsh Sudano-Sahelian environment, as well as the physical mechanisms at work in the system that can lead to more robust yields.

Over the last two years, data were collected on soil moisture and temperature, climate, water retention, infiltration rates, crop yield parameters, handheld normalized difference vegetation index (NDVI), leaf water potential, and leaf area index (LAI). In 2012 and 2013 at these long-term sites, there was significantly higher yield of both peanut and millet in shrub-associated plots compared to sole crop plots. At Keur Matar, the effect of shrub presence on peanut grain yield and millet panicle mass was as large as the effect of the maximum fertilizer input on the sole-crop plots. The data also show a decreased level of water stress in shrub-associated crops with, in some cases, significantly lower midday water potential, and increased normalized difference vegetation index (NDVI). Water-retention measurements reveal that the soils under the shrub are able to provide significantly more water to plants at matric potentials between field capacity and a pearl millet stress threshold of -0.5 Mpa. Inverse solutions in HYDRUS 1-D were performed with automated mini-disc tension infiltrometer data, and despite a non-uniqueness of the solution, the shrub-associated soils yielded lower saturated hydraulic conductivity values overall. Differing soil properties as well as the mechanism of hydraulic redistribution (HR) within the shrub root zone have been shown to exist and may serve to decrease water stress in associated plants.

An isotopic tracer study investigating hydraulic redistribution is currently under way to determine the fate of deuterium-labeled water applied to deep shrub roots during a hard drought stress. Effects of the shrub rhizosphere and biomass additions on the soil properties surrounding the shrub canopies are profound in these nutrient-poor soils, and many of the traditional agro-forestry mechanisms of nutrient retention, shading, and erosion reduction hold true. One thing that has not been observed, however, is any negative effect of the shrub competition on surrounding crops.

These findings build on work that was completed in 2004 at the site, but point to significant changes in soil properties under the shrub canopies. Adoption of this agro-forestry technique is possible over wide swaths of the Sahel, even with the limited resources that local subsistence farmers possess.

Amendment Effects on Arsenic Uptake in Paddy Rice—Deciphering the Regulating Mechanisms

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Rice is the primary food source for people in South and South-East Asia, an area heavily affected by natural arsenic (As) contamination of soil and water. Mitigating the arsenic uptake in rice requires an understanding of how different management practices influence the regulating mechanisms in the rhizosphere that are responsible for As migration from soil into rice roots. We approach this challenge through coupling spatially resolved analyses with time series and end-point bulk measurements of As in the solid/aqueous phase in the soil and in the plant.

In a pot trial with As-contaminated soil from Cambodia, charred rice straw, charred rice husks, and gypsum were tested as amendments to limit the As uptake in rice. Both types of char decreased the As concentration in rice straw and grain, whereas gypsum had no effect or even increased the As uptake slightly. The effect was greatest with the charred straw. Preliminary results from synchrotron XRF mapping and bulk XANES analyses suggest that As adsorption to sulfhydryl groups on the char, in combination with sulfide precipitation, increased As partitioning to the solid phase in the char treatments. Furthermore, the solubilization of As was delayed in the charred straw treatment, suggesting that the timing of As release relative to plant growth stage could be another contributing factor. The functional differences between the chars were further investigated in batch reactors where As, Fe, and S solubility and chemical speciation over time was analyzed and coupled to microbial metabolism, as measured through isothermal microcalorimetry.

Our data highlights the importance of a temporally and spatially resolved, multiple-scale approach to understanding complex soil systems, such as the paddy rice environment. Furthermore, it suggests that biochar could limit the As uptake in rice through preferential stimulation of sulfate-reducing bacteria, delayed As release, and increased As adsorption.

The Implications of Soil-Moisture Spatial Scaling Structure for Sampling of the Soil Moisture Field

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The characteristics of soil-moisture spatial patterns are fundamental to understanding the dynamics of soil moisture and soil-moisture-dependent processes in space and time. The soil-moisture sampling strategies we employ and the soil-moisture spatial patterns that we perceive are affected by each other. The previously reported spatial scale-invariance of soil moisture implies great potential for improving the accuracy and efficiency of soil-moisture sampling designs. This research aims to verify and describe the spatial scale invariance of soil moisture at the field scale with point measurements. Soil-moisture surveys were conducted at the scale of one to hundreds of meters at the OSU Range Research Station, Marena, OK. Spatial variance and autocorrelation of soil moisture will be calculated and compared at multiple scales. The implications the soil-moisture scaling characteristics for improving soil-moisture sampling designs will be discussed.

The Impact of Winter Cover Crop Development on Nitrate Leaching: Combining Field Observations with Computer Modeling

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Groundwater nitrate pollution poses a serious challenge in intensively managed agricultural systems. Therefore, it is important to develop crop management practices that limit nitrate transport past the root zone. In California, leaching can be significant during winter months, when fields are commonly left fallow, evaporation is low, and precipitation can be high. In some systems, cover crops grown during the winter have been shown to reduce leaching by immobilizing nitrate in the biomass and/or reducing percolation of water through the soil. The effectiveness of cover crops in reducing nitrate leaching is likely to be highly dependent on the development of the root system, along with the timing and magnitude of winter precipitation. To investigate this issue, we conducted a field study at the U.C. Davis Sustainable Agriculture Facility to quantify water and nitrate movement within and below the root zone, along with cover crop canopy and root system development.

The two cover crops used in the study were triticale (*x Triticosecale*), a grass species that produces a fibrous root system, and bell bean (*Vicia faba*), a legume that produces a taproot system and fixes N. The two cover crops were grown separately, and fallow fields served as a control. Soil-water movement was measured through a network of soil-moisture sensors and tensiometers placed at depths ranging from 30 to 210 cm. These data were used to calculate soil hydraulic properties in the different soil layers and to quantify both upward and downward water fluxes below the root zone. Soil solution was collected to measure soil nitrate concentration using (1) suction cup soil-solution samplers placed at the same depths as the tensiometers and (2) equilibrium tension lysimeters, installed below the root zone (125 cm). Nitrate leaching was calculated directly from the volume of water collected by the equilibrium tension lysimeters, as well as from the calculated water fluxes and nitrate-concentration measurements obtained from soil-solution samples. Roots were obtained from washed soil cores taken at 3-4 times during the 2012-2013 and 2013-2014 winter seasons. Washed roots were imaged and root-length density was quantified using the WinRhizo imaging software. Because of the bell bean's poor establishment and relatively slow growth, weed growth was significant, with 48-90% of total biomass consisting of weeds. Compared to the bell-bean treatment, triticale grew significantly faster, deeper (~ 125 cm, compared to 90 cm) and produced larger root systems. By the end of the cover-crop season, both treatments reduced soil nitrate concentrations within their respective rooting depths; however, triticale was more effective (95% reduction in 0-125 cm for triticale, versus 85% reduction in 0-90 cm for bell bean). Furthermore, nitrate leaching (defined as total nitrate that moved past 125 cm during the season) was lowest in the triticale treatment, while bell bean increased nitrate leaching slightly over the winter fallow control.

These results suggest that while both treatments depleted soil nitrate, triticale's deeper root system and faster growth resulted in less leaching and made it more effective as a nitrate catch crop. Efforts are currently under way using Hydrus 1D/2D to identify root-system characteristics that have the greatest impact on nitrate movement past the root zone, and to identify management practices that minimize nitrate leaching while avoiding undesirable effects, such as inadequate soil moisture for establishing the following cash crop.

Influence of Diesel Contamination in Soil on the Growth and Dry Matter Partitioning of *Lactuca Sativa* and *Ipomoea Batatas*

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The effects of diesel soil contamination on the growth and dry-matter partitioning in *Lactuca sativa* and *Ipomoea batatas* were studied in a greenhouse pot experiment at two concentration ranges (0-30 mL and 0-6 mL diesel/kg soil) for 14 weeks. The result indicated that whole plant biomass, plant heights, number of leaves, root lengths, and the leaf chlorophyll in the two species were negatively correlated with increasing diesel concentrations. The critical concentrations of diesel associated with 10% decrease in plant growth were 0.33 mL for lettuce and 1.50 mL for sweet potato. Thus, the growth of lettuce in diesel-contaminated soil was more sensitive than the vegetative growth of sweet potato. The pattern of dry-matter partitioning in both species was similar. In the 0-6 mL, diesel-concentration contamination range, allocation of dry matter to the shoot system was favored, resulting in a high shoot: root ratio of 4.54 and 12.91 for lettuce and sweet potato, respectively. However, in the 0-30 mL diesel-concentration range, allocation of dry matter to the root was favoured, which may have been an adaptive mechanism in which the root system was used for storage in addition to increasing the capacity for foraging for mineral nutrients and water. Although lettuce accumulated more metals in its tissue than sweet potato, the tissue mineral nutrients in both species did not vary to a great extent. The critical diesel concentration for toxicity suggested that the cause of mortality and poor growth of sweet potato and lettuce grown in diesel-contaminated soil is direct toxicity of diesel hydrocarbons.

Hierarchical Clustering and Principal Component Analysis as Tools for Classification and Selecting Representative Field Sites

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Selection of representative sites for field investigations is usually based on a set of multiple criteria—quantitative and qualitative characteristics and attributes describing (for example) the site soil, geology, topography, climate, hydrology, and biome conditions. Although these criteria are generally dependent on each other, one has to consider that the regional-scale ecological systems are hierarchical systems, containing many levels of mutually interacting subsystems. The LBNL Subsurface Biogeochemistry Scientific Focus Area DOE project is in the midst of establishing a second field study site that has characteristics complementary to the existing site near Rifle, CO. A list of site candidates included over 20 sites in different regions of the USA. In this paper, we explore the application of a combination of the Hierarchical Clustering and Principal Component Analysis (HCPC) as a tool for classification and selecting representative field sites.

Our approach is based on a combination of exploratory data analysis, principal component methods, and hierarchical clustering and partitioning, to enrich the site-selection procedure. Principal component analysis is used as a preprocessing step for clustering in order to reduce the level of complexity in decision making—in other words, to "denoise" the data and to transform categorical data into continuous or balanced groups of site characteristics. The hierarchical tree is also used to visualize the principal component representation and the partition of data, which allows one to better understand the groups of site characteristics and the sites. In this analysis, we used quantitative site characteristics (including monthly and annual temperature, annual precipitation, elevation, supplementary and quantitative variables), site geographical coordinates, and categorical variables (including climate, soil/rock, biome, region, and watershed characteristics). The sites were also assigned a series of weighting factors, based on the level of priority of investigations (i.e., an expert opinion). The results of sites classification are shown using dendrogram plots, presenting several levels of the hierarchical classification of sites. A proper classification of the field sites is critical for accomplishing one of the primary DOE missions—planning basic research to understand the complex physical, chemical, and biological phenomena of contaminated sites and climatic investigations.

Rethinking Nutrient Limitation in Soils: Linking Soil Carbon Cycling to Phosphorus Availability with Biological Stoichiometry Theory

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The turnover of terrestrial carbon (C) in soil and plant litter pools is often represented in ecosystem and decomposition models as a function of nitrogen (N) availability (e.g., C:N ratios). However, an emerging body of work indicates an important and under-represented role of phosphorus (P) in determining C turnover in soils. The results of our recent global meta-analysis suggest that P availability is linked with microbial metabolism across terrestrial and wetland ecosystems. We have also found that soil C cycling is more closely coupled with soil phosphorus than N in ecosystem studies across wetland types on the Eastern U.S. seaboard, and in rice fields in California spanning a wide range of soil C concentrations. Importantly, these observations of phosphorus limitation in soil C turnover were made in wetlands where vegetation was limited by N, and similar observations have recently been made in grasslands and forest soils. These patterns may arise as the result of underlying mechanisms described by Biological Stoichiometry Theory, founded on the Growth Rate Hypothesis (GRH). This hypothesis describes relationships between cellular metabolic rates and P concentrations as arising from the dependence of growth rates on P-rich ribosomal RNA needed for protein synthesis, while biomass accumulation depends on N-rich proteins. Extended across orders of magnitude in organism size, the GRH accounts for the greater demand for P of small, fast-growing soil microbes relative to terrestrial plants, suggesting different nutrients could limit primary productivity and decomposition in soils. While our current research seeks to explore how soil P availability may be linked with functional differences in wetland soil microbial communities, we solicit feedback and collaboration to improve our understanding of the broader processes and their implications for global soil C cycling. Recently published datasets on global soil phosphorus concentrations and C content of soil microbes suggest adequate data may be available to incorporate these processes into global ecosystem models, although further empirical work may be needed to better characterize and parameterize the relevant processes.

Modeling the Optimal Phosphate Fertiliser and Soil Management Strategy for Crops

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The readily available global rock phosphate (P) reserves are set to run out within the next 50-130 years, causing soils to have a reduced P concentration which will affect plant P uptake. Careful use of this finite resource in agriculture systems is clearly warranted. We therefore present a model which searches for optimal fertilizer and soil-management strategies for crop production while maintaining a sustainable plant P uptake. In this paper, we present the results for wheat; however, the model is adaptable for other types of crops, subject to root-structure data being available. The model describes the development of the phosphate and water profiles within the soil space. Current cultivation techniques such as ploughing and a reduced till gradient are simulated along with fertilizer options to feed the top soil or below the seed. By trying to minimize the amount of fertilizer used and achieving a sustainable level of P uptake, we create a multi-objective problem, which is solved using optimization algorithms. We find that a well-mixed soil (ploughing) is critical for optimal P uptake and provides the best environment for the root system. The combination of modeling and experimental data provides useful predictions for site-specific locations.

Interconnections among Aggregate Structures, Organic Matter, and Microbes in Rhizosphere-Dominated Soils

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Nearly ideal conditions for soil-aggregate formation and stabilization exist in the rhizosphere. As fibrous roots grow, they exert pressures and locally dry the soil, causing soil particles to be pushed and drawn together, at the same time that exudates and rhizodeposits support a diverse microbial and faunal community. Roots and the hyphae of associated mycorrhizal fungi serve as a flexible latticework that enmeshes and stabilizes larger aggregates. Because root turnover often occurs within the inner spaces of soil aggregates, the decomposition process leads to the formation and stabilization of microaggregates within macroaggregates, and development of an aggregate hierarchy. The resulting physical structure feeds back to impact decomposer access to substrates, air, water, and nutrients, thereby affecting decomposition and soil carbon dynamics. In past work (Jastrow et al., 1998, Soil Biol. Biochem. 30:905-916), we used path analysis to demonstrate that the recovery of a stable macroaggregate structure in restored grassland was driven by the direct and indirect effects of roots and mycorrhizal hyphae, with lesser relative contributions from microbial biomass, soluble carbohydrates, and soil organic matter. But the interactions among aggregate structures, soil organic matter, and the microbial community lead to more complex interconnections and feedbacks. Here, we reverse the conceptual focus of our path analysis approach to explore (1) the integrated roles of macroaggregate structure as the habitat for soil microbes and as a mechanism for the physical protection of particulate organic matter, and (2) the outcome of that interplay on the accrual of mineral-associated organic matter. We also investigate the multivariate relationships among the microbial community and the physical distribution of particulate and mineral-associated organic matter forms within the hierarchical structures of grassland soils.

Predicting Saturated Hydraulic Conductivity by Soil Parametric and Morphological Properties

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Many studies have been conducted to describe soil saturated hydraulic conductivity (Ks) by readily available soil properties such as bulk density, texture, porosity, pore-size distribution, and so on. However, while soil morphological properties have a strong effect on Ks, studies aimed at describing the relationship between Ks and soil morphological properties (such as type, size, and strength of soil structure; type, orientation and quantity of soil pores and roots; consistency; plasticity, etc.) are rare. This study aims to evaluate soil morphological properties along with soil parametric properties to predict Ks. The study was conducted on paddy soils and adjacent grasslands on Kızılırmak Township (near the town) of Cankırı Province. Undisturbed soil samples (15 cm length and 8.0 cm id.) were collected at sixty randomly selected sampling sites from topsoil (0-15 cm) and subsoil (15-30 cm) (120 samples) with a tractor operated soil sampler. Synchronized disturbed soil samples were taken from the same sampling sites and depths for basic soil analyses. Saturated hydraulic conductivity was measured on the soil columns using a constant-head permeameter. Following the K_s measurements, the soil columns were left to drying to field capacity and penetration resistance was measured on the columns, then the soils were disturbed and morphological properties of soils (soil structure, pores, roots, consistency, plasticity, and stickiness) were described by standard soil description charts used in soil survey studies. In addition, soil texture, percent gravel, bulk density, pH, field capacity, wilting point, cation exchange capacity, specific surface area, aggregate stability, organic matter content, and calcium carbonate were measured on the synchronized disturbed soil samples. The K_s was predicted from the soil morphological properties by stepwise multiple linear regression and correlation analyses. Soil structure class, stickiness, pore-size, root-size, and pore-quantity contributed to the Ks prediction significantly. Soil morphological properties, readily available in soil survey databases, may be used along with basic soil properties in predicting K_s.

Relationship between Soil Water Potential and Sorptivity in a Clay Soil

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Sorptivity, the most important variable affecting management of early infiltration processes, is significantly influenced by the initial water content (in addition to several other soil properties). Numerous studies have been conducted to analyze the effect of soil water content on sorptivity. However, studies focused on the response of sorptivity to soil water potential are rare. This study analyzed the interaction between soil water potential and sorptivity in clay soils. Seventeen undisturbed soil samples (5 cm id and 5 cm length) were taken from 0-15 cm soil depth. Sorptivity was measured with a mini disc infiltrometer at different soil water pressures equilibrated in a pressure plate apparatus ranging from 20 to 1500 kPa. In general, decreased soil water pressure resulted in increased sorptivity down to -100 KPa, while further decreases in soil water pressure affected sorptivity adversely.

Relationship between Spatial Resolution and Accuracy of Predictive Maps Comparing Soil Survey Geographic (SSURGO) Database Aggregation and Terrain Attribute Soil Mapping (TASM)

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The success of predictions when modeling hydrology depends on the accurate representation of spatial and temporal variability of external major drivers such as weather, land use, land management, geomorphic surface, and soils. The evolution of soil models capturing the spatial and temporal variability has recently focused the attention of soil scientists on current soil information, especially soil properties as they relate to hydrologic modeling. The challenge for pedologists is to accurately and completely represent the spatial variability of soil properties and relate this variability to scales. For hydrologic modeling purposes, this means that soil morphological differences need to be viewed from the perspective of hydrologic processes leading to the generation of soil functional hydrologic property maps with a focus on commonality rather than morphological differences. The overall goal is to assess the role of the resolution of predicted soil properties on simulated hydrological response. The study site is Hall Creek watershed approximately 56 km2 in area upstream of the USGS gauge near St. Anthony (USGS id 03375800) located in Dubois County in southern Indiana. SSURGO soil property maps and terrain attribute soil maps (TASM) at 10, 30 and 90 m pixel sixe are used as input to Distributed Hydrology Soil Vegetation Model (DHSVM) to investigate the role of the resolution of predicted soil properties on simulated hydrological response. There were no significant differences in the mean annual flow between the 10, 30 and 90 m model pixel resolution with the exception of the SSURGO 90 m. The R-B flashiness index and annual maximum flow increased significantly with model resolution for both TASM and SSURGO soil maps, while annual minimum discharge decreased. The fact that stream flow metrics were not influenced by soil pixel aggregation can be related to the contribution of each model input to the stream flow. In this simulation, soil depth varied only between 0.7 and 2 m throughout the watershed thus its contribution to the stream flow dynamics is relatively small compared to evapotranspiration. The use of continuous raster soil depth maps derived from terrain attribute soil mapping (TASM) is in general advantageous to the raster soil depth maps derived directly from gridded SSURGO polygon soil depth maps especially for 90m pixel resolution.

A Model for Estimating Soil Thermal Conductivity from Texture, Water Content, and Bulk Density at Moderate Temperature

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Soil thermal conductivity (λ) models are needed frequently in studying coupled heat and water transfer in soils. Several models are available, but some are complicated and some produce relatively large errors. In this study, we introduce a simple model for estimating λ from soil texture, bulk density (ρ_b), and water content (θ) in the entire water content range. The model parameters were determined by fitting the model to heat-pulse measurements of $\lambda(\theta)$ on seven soils of various textures, and the model performance was evaluated with additional $\lambda(\theta)$ data from heat-pulse method and literatures. The results showed that the model was able to express the general trend of $\lambda(\theta)$ curves from oven-dry to saturation at fixed ρ_b values. When ρ_b was varied, the errors of λ estimates were within 25% of the measurements, with soil texture ranging from sands to silty clay loam. Further validation with literature datasets indicated that the predicted λ data agreed well with measured values, with RMSEs less than 0.15 W m^{-1} K^{-1}, and the model produced compatible results with the Lu et al. (2007) model. The new model has the potential for studying heat movement in soils and can be incorporated into numerical algorithms for describing coupled heat and mass-transfer processes.

Soil and Root Microbiota of a Field-Grown Tomato at Various Spatial, Temporal, and Pathological Scales

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Few studies have utilized next-generation sequencing to profile the microbial communities in intensively managed agroecosystems. The goal of the study presented here is to gain a DNA-based understanding of the bacterial and fungal community structure of agricultural soils in relation to crop performance and soilborne diseases. Our specific aims were as follows: (1) to describe the microbial diversity associated with soils and plant roots in processing tomato fields, (2) to demonstrate the impact of field location and management on this microbial diversity, and (3) to reveal correlations between community structure, abundance of soilborne pathogens, root health, and fruit yield.

Over a three-season period, experimental plots were set up and sampled in a total of six commercial processing tomato fields in the Sacramento Valley. Each plot featured up to nine treatments consisting of single or combined applications of the following chemicals and biologicals (with active ingredient): Vapam (metam sodium), Quadris (azoxystrobin), Ridomil Gold SL (mefenoxam), Tenet (*Trichoderma asperellum* and *T. gamsii*), SoilGard (*Trichoderma virens*), Serenade Soil (*Bacillus subtilis*), Actinovate (*Streptomyces lydicus*), Soil System I (unspecified blend of beneficial bacteria), and composted chicken manure. Treatments were delivered to the soil by one-time incorporation prior to planting (composted chicken manure) or by injection at one or more times through subsurface drip lines (all other treatments). Bulk and rhizosphere soil samples were collected at various time intervals during the growing season up until harvest. Total DNA was extracted from soil samples and used to amplify bacterial 16s rRNA gene V4 regions and fungal ITS1 regions, which were mass-sequenced on the Illumina MiSeq platform. Amplicon sequences were analyzed using the QIIME pipeline for microbial community analysis.

Analysis of the data revealed a significant field effect: in PCoA plots, soil samples from individual fields clustered closely together. This was true for both bulk and rhizosphere samples. There also was a temporal effect in that microbial community composition changed over the span of the growing season. The data also showed significant differences between the microbial communities of bulk and rhizosphere soils. Rhizosphere soil samples exhibited a lower diversity compared to bulk soil and appeared enriched for the bacterial genera *Bacillus*, *Pseudomonas*, *Streptomyces*, *Olivibacter*, *Sphingobium*, and *Agrobacterium*. Also enriched in the tomato root were the fungal species *Pyrenochaeta lycopersici*, *Plectosphaerella cucumerina*, *Rhizoctonia solani*, *Fusarium oxysporum*, and *Colletotrichum coccodes*. All of these are known plant pathogens of tomato, causing corky root, greenhouse wilt, seedling damping-off, Fusarium wilt/crown-root rot, and anthracnose, respectively. These results confirm the notion that tomato plant roots attract tomato pathogens.

The strong field effect complicated our analysis of the impact of different treatments on microbial community composition, in that treatment effects could not be readily identified by averaging data over all fields. However, preliminary analysis of per-field data suggests that microbial community composition was not significantly impacted by our treatments, and that microbial communities in agricultural soils are resilient to short-term single-season inputs. With respect to fruit yield and disease severity, only the composted chicken-manure treatment showed an improvement: it had 25-40% higher yields and clearly lower levels of leaf necrosis compared to the nontreated control. This positive effect on tomato plants in the absence of obvious changes in microbial community structure suggests that composted chicken manure provided a nutritional benefit to the roots.

Improving Arsenic Phytoremediation Efficiency under Heterogeneous Field Conditions: Effects of Fertilizer on Brake Fern Arsenic Accumulation and Biomass Production

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Arsenic is toxic at low concentrations and widespread in the environment, making arsenic soil contamination a global issue. Historic and ongoing activities including mining of metal ores, pesticide use, and coal combustion have resulted in elevated arsenic concentrations in soils. *In situ* soil rehabilitation is challenged by soil heterogeneity and heterogeneous distribution of contaminants. Phytoremediation with the arsenic hyperaccumulating fern *Pteris vittata* L., or Chinese brake fern, is an emerging technology to remediate soils with shallow arsenic contamination. Mechanisms of arsenic uptake and accumulation in the brake fern have received attention in numerous greenhouse and hydroponic experiments. However, the fern's performance under field conditions remains poorly understood. At remediation sites, environmental variables that are only partially controllable, including temperature, precipitation, and soil quality, can affect both fern and arsenic behavior. Published estimates of arsenic phytoremediation times using *P. vittata* are on the order of decades. More research is needed to optimize *P. vittata* performance, improve remediation times, and thus develop more successful *in situ* remediation methods.

The objective of this study is to develop a new methodology to increase *in situ* arsenic phytoremediation efficiency and decrease remediation time. We present results of an ongoing experiment to assess fertilizer impact on brake-fern biomass production and arsenic uptake under field conditions. The study site is an abandoned railroad right-of-way with sandy loam soil moderately contaminated with arsenic (85.5±8.8 ppm) and characterized by a Mediterranean climate. A total of 1,600 *P. vittata* ferns were planted in February 2013, spaced 30 cm apart (11 ferns m^{-2}), with 200 or 400 ferns per subplot. To compare effects of inorganic and organic fertilizers, five amendments were applied to separate fern subplots, with applications designed to deliver equivalent nutrient amounts based on standard agricultural rates. Amendments included ammonium sulfate (inorganic N), blood meal (organic N), rock phosphate (inorganic P), bone meal (organic P), and compost (organic application of many nutrients). Results of fern arsenic accumulation and harvested biomass after 8 months of growth, and estimates of arsenic removal from soil, will be presented. Soil heterogeneity will be shown through localized gradations in soil texture and bulk density, illustrating the complex nature of researching and remediating soils characterized by fill. Preliminary results suggest that compost is most effective at increasing both fern arsenic uptake and biomass production.

Practical Application of Chaotic Advection to Groundwater Remediation

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Laminar flow limits mixing in groundwater remediation. As a result, biogeochemical reactions between injected treatment solutions and subsurface contaminants are confined to a narrow interface zone between the plume of injected fluid and the surrounding contaminated groundwater. Because it enhances mixing, plume spreading is a key process in groundwater remediation that has gained considerable attention in recent years. Nonuniform flow, resulting from aquifer heterogeneity, generates plume spreading passively. Chaotic advection, in which the trajectories of fluid parcels exhibit sensitive dependence on initial conditions, generates plume spreading actively. As an active process, chaotic advection offers the potential to improve groundwater remediation through engineered manipulation of the groundwater velocity field to generate stretching and folding of fluid elements. This presentation will report a series of simulations and experiments that represents the first demonstration—to our knowledge—of plume stretching and folding in laminar, irrotational flows without reinjection. Simulations using both analytical and numerical models have (1) demonstrated the presence of chaotic advection, (2) revealed how the characteristics of chaotic advection depend on aquifer heterogeneity, and (3) predicted faster rates and increased extent of reactive transport. In parallel, laboratory experiments using a Hele-Shaw apparatus have confirmed the feasibility of plume stretching and folding, and have provided insight into the interplay between chaotic advection, which generates plume structure, and dispersion (here Taylor dispersion), which destroys plume structure. This approach sidesteps the recognized difficulty in simulating dispersion. These experiments are the first step toward application of chaotic advection to groundwater remediation at field sites.

Estimating Leaching of Water and Nitrate below the Root Zone of Multiple Crops Using a Combination of Field Instrumentation and Modeling

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There is growing concern over the shortage of fresh water, the need for sustainable agricultural production, and the risk of soil and groundwater pollution. All these concerns require the optimization of fertigation/irrigation practices, in order to maximize their application efficiency and minimize fertilizer losses through leaching to groundwater. To optimize irrigation/fertigation of citrus, it is essential that irrigation water and fertilizers are applied at the rate, place, and time that ensure maximum yield and fruit quality, while leaching of water and salts (nitrate) to groundwater is minimized, and buildup of salts in the root zone of trees is avoided. However, applied irrigation water and dissolved fertilizer, as well as root growth and associated nutrient and water uptake, interact with soil properties and nutrient sources in a complex manner—such that a coupling of experimentation and modeling is required to unravel the complexities resulting from spatial variations in soil texture and layering often found in agricultural fields. We have developed a combination of field instrumentation and modeling to calculate downward fluxes of water and nitrate at the scale of a single tree, plot, and orchard. By calculating the gradients in water potential across a soil layer deep below the root zone, with known soil hydraulic properties, the daily fluxes of water and nitrate (measured concentrations) can be calculated using the Darcy equation. Further simplification of the necessary instrumentation used in this method would make it a reliable and attractive tool for quantifying leaching of water and nitrate below the root zone of croplands under any management practices. This method is being tested in various crops in California, including tomato, citrus, almond, pistachio, and walnut. We will present experimental approaches that provide the necessary data on soil moisture, water potential, and nitrate concentration, as well as multidimensional modeling of unsaturated water flow and solute transport to calculate fluxes of water and nitrate under various orchards and various management practices. These results will be used to evaluate and optimize irrigation and fertility management practices for multiple locations, crop types, and irrigation systems.

Soil Water Content Variability in the 3D "Support-Spacing-Extent" Space of Scale Metrics

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Knowledge of soil water content (SWC) variability provides important insight into soil functioning, and is essential in many applications. This variability is known to be scale-dependent, and divergent statements about the change of the variability magnitude with scale can be found in the literature. We undertook a systematic review to see how the definition of scale can affect conclusions about the scale-dependence in SWC variability. Support, spacing, and extent were three scale metrics. We found six types of experiments in which scale was changed. With data obtained without a change in extent, the scale change in some cases consisted in the simultaneous change of support and spacing, and the power law decrease in variance with support increase was found. Datasets that were collected with different support or sample volumes for the same extent and spacing showed a decrease in variance as the sample size increased. A variance increase was common when the scale change consisted of a change in spacing without any change in supports and extents. An increase in variance with the extent of the study area was demonstrated with data an evolution of variability with increasing size of the area under investigation (extent) without modification of support. The variance generally increased with the extent when the spacing was simultaneously changed. Finally, the decrease in variability was noted for changes in extent for a given support without modification of spacing. All above trends were holding up to some threshold scale metric value. We noted that a set of hyperplanes can be used to depict the scale dependencies in the space of scale metrics. Slopes, thresholds, or both appear to be preserved as SWC changes. Overall, published information on the effect of scale on soil water content variability in the 3D space of scale metrics did not contain controversies in qualitative terms. However, there were substantial differences in quantitative terms, which might reflect site-specific differences in soil water content controls and scale change methods. Since both local and nonlocal controls on SWC appear to be scale-dependent, scale metrics have to be matched for SWC and for controls to evaluate the effect of the controls on SWC variability.

Nurturing the Link between Resilience, Complexity and Sustainability at the Landscape Scale

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A goal of sustainable management practices is to maintain the system's identity and ability to persist over multiple production cycles. However, many management interventions, particularly in agricultural landscapes and managed forests, simplify the system by, for example, reducing the number of species or decreasing spatial and structural heterogeneity. Such simplifications can reduce the capacity of the system to absorb and recover from disturbance, reducing its resilience and thus its sustainability. This presentation explores the relationship between complexity, resilience, and sustainability, and discusses how a complex systems approach to management might better nurture this relationship. Through an expanded vision of the landscape as a complex, human-environment system, managers can devise management plans that more adequately maintain the complex structure and functioning of the landscape necessary for a healthy and sustainable environment.

Soil Salinity Measurement and Habitat Sustainability in Brackish Seasonally Managed Wetlands

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Seasonally managed brackish wetlands in the San Joaquin Basin of California are an important resource for migratory waterfowl on the Pacific Flyway. These wetlands, deprived of floodwaters from the San Joaquin River after construction of the Friant Dam and the Central Valley Project, now rely on the importation of a higher salinity water supply from the Sacramento San Joaquin Delta. Salinity management is essential for the long-term sustainability of these brackish wetlands—requiring routine salinity mapping and soil-profile salinity assessment. The complex hydrology and the high clay content of the soils beneath many of these wetlands challenge both tasks. Soils desiccated during the dry summer crack and leave fissures often extending more than ½ meter below the soil surface. Fall flooding of these seasonal wetlands dissolves effloresced salt from the soil surface that are washed into these cracks, creating a unique mottled near-surface stratigraphy. This creates challenges for soil-salinity mapping using electromagnetic survey techniques. In addition, ponded water held for longer in adjacent seasonal wetlands can cause higher rates of salination in seasonal wetlands that are drawn down early, as well as cause greater salt efflorescence. The impact of this phenomenon is realized during fall flood-up the following year, resulting in high salinity levels in ponded water and higher rates of salt precipitation in the soil matrix. This creates a requirement for more frequent soil surveys and wetland impoundment management on a subregional scale. This paper takes a systems approach to soil-salinity measurement and assessment in this complex, and suggests a new approach to wetland soil-salinity management.

Soil Organic Carbon Responses to Multi-Nutrient Addition

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Humans have dramatically altered the cycling of biologically relevant elements, such as nitrogen (N), phosphorus (P), and potassium (K), on Earth. Although soils are an important reservoir of fixed, organic carbon (C), the effects of nutrient enrichment on this significant C stock remain uncertain. In particular, whether the effect of nutrient addition on microbial decomposition of soil organic matter differs when nutrients are added singly or in combination is still unclear. We hypothesized that N addition alone would increase soil C stocks due to the inhibitory effects of N on microbial oxidative enzyme activity. Furthermore, we hypothesized that these inhibitory effects would be negated with the addition of non-N nutrients that alleviate microbial nutrient limitation, leading to increased decomposition (and no change in soil C stocks). To address these hypotheses, we sampled soil organic C from a global network of >60 grassland sites that have received full factorial additions of N, P, and K (these sites are experimental sites of the Nutrient Network). Following three years of nutrient addition, there was a significant N*P*K interaction effect on total soil C ($p = .012$). Total soil C increased significantly when N was added alone, as well as in combination with K and P+K ($p = .049$, .044, and <.001, respectively). Furthermore, N+K addition significantly increased soil C within the P addition treatment ($p = .020$) and K significantly increased soil C within the N+P addition treatment ($p = .018$). These results were in partial support of our hypotheses. Although we did detect N addition effects alone, we also observed treatment effects in combination with K and K+P. This may be due to the acidifying effects of the micronutrient addition that accompanied the K treatment.

Altogether, our results suggest that while N addition and N+K (+ micronutrients) increases soil C stocks, these effects are partially negated when combined with P addition. Assessing soil C responses to multi-nutrient addition across >60 grassland sites worldwide advances our general understanding of soil C responses to nutrient enrichment. By identifying these global patterns, as well as site-specific deviations, we will inform future efforts to predict soil C sequestration potential across broad spatial scales on our increasingly fertilized planet.

Decreasing Fertilizer Use by Optimizing Plant-Microbe Interactions for Sustainable Supply of Nitrogen for Bioenergy Crops

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Nitrogen (N) is an essential component of DNA and proteins, and consequently a key element of life. N often is limited in plants, affecting plant growth and productivity. To alleviate this problem, large amounts of N-fertilizer are added, which comes at a high economic price and heavy energy demand. In addition, N-fertilizer also significantly contributes to rising atmospheric greenhouse gas concentrations, nutrient leaching, and (consequently) hypertrophication—and is thus highly undesirable.

As a sustainable alternative, our research focuses on optimizing interaction between plants and diazotrophic bacteria, which could provide adequate amounts of N to the host plant. We investigated microbes associated with tobacco (*Nicotiana tabacum*) and switchgrass (*Panicum virgatum*), considered as potential energy crops for bioenergy production. Several bacterial isolates with representatives from Alphaproteobacteria, Gammaproteobacteria, Actinobacteria, Bacteriodetes and Bacilli were obtained from the roots, leaves, rhizoplane, and rhizosphere of these plants. We also isolated several endophytes. We are at present investigating the physiology of these isolates—substrate range, temperature, and salinity requirements for growth. As shown by PCR amplification of *nifH*, several of them are potential N_2-fixing bacteria, which was also confirmed quantitatively by measuring nitrogenase activity. To confirm the N_2-fixing activity of isolated endophytic diazotrophs, we used fluorescent-tagged strains to re-infect aseptic *Nicotiana tabacum* and *Panicum virgatum* seedlings by different imaging techniques. In addition, we also investigated utilization and transformation of root exudates by rhizobial diazotrophs. Currently, metabolite profiling of the exudates is in progress to identify possible signaling molecules and carbon sources secreted by the plant to promote colonization of such strains. Together, this understanding is necessary for the development of eco-friendly, economically sustainable energy crops by decreasing their dependency on fertilizer.

Soil Systems for Up-scaling Saturated Hydraulic Conductivity (Ksat) for Hydrological Modeling

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The spatial variability of soil hydraulic conductivity (Ksat) impacts the performance of hydrological models. This is especially critical for distributed hydrological models as it controls the rate of water movement not only vertically but also laterally and across the landscape. Soil Systems is one of the approaches for assigning the proper Ksat values in order to represent water movement at watershed scale. The Soil Systems approach allows the up-scaling of soil processes and functions by characterizing soils that are representative of larger areas. Ksat values calculated from point measurements and adjusted based on nested wells/piezometers as well as flume discharge data from a small catchment (1st order) were used as input to the Distributed Hydrological Soil Vegetation Model (DHSVM) to predict the discharge for a HUC12 watershed. The performance of the DHSVM was assessed based on Nash-Sutcliffe model efficiency, which compares the observed and simulated daily stream flows. A Nash-Sutcliffe model efficiency of 0.52 indicates good performance by the model. This Nash-Sutcliffe model efficiency was very good for early spring precipitation events (0.72) and poor for summer events (0.18). The poor performance for summer events is expected, given the evapotranspiration demands and the localized nature of summer precipitation events. Despite this, the good performance overall and very good performance of the model for early spring precipitation events without model calibration illustrates the advantage of using a Soil Systems approach for up-scaling not only soil processes and functions, but also hydrological processes.

Miracle in the Vadose Zone of Onsite Wastewater Treatment Systems: Understanding Soil Processes Complexity in Remediating Wastewater-Borne Contaminants

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Understanding the fate and transport of contaminants in the vadose zone of onsite wastewater treatment systems (commonly called septic systems) is crucial to protect groundwater and surface water quality. In areas with shallow groundwater such as Florida, there is increased connectivity of ground- and surface-water, with groundwater being a significant contributor of base flow in streams, rivers, and estuaries. The presence of porous sandy soils further aggravates transport of water and chemical constituents present in septic tank effluent (STE). For example, our data shows that about 47% of applied water from STE and rainfall was recovered at 60 cm below drainfield. This implies that a chemical constituents present in STE, if not attenuated in the vadose zone of septic systems, can potentially move to shallow groundwater and eventually end up in surface waters.

The objective of this study was to investigate the biophysical and hydrologic controls on transport of nitrogen (N), phosphorus (P), pharmaceuticals, and hormones in the vadose zone of two conventional systems (drip dispersal, gravel trench) and an advanced system containing aerobic and anaerobic medias.

These systems were constructed as part of a Florida Department of Health N reduction study using two rows of drip pipe (37 emitters/mound) placed 0.3 m apart in the center of 6 m × 0.6 m drainfield. Each system received 120 L of STE (equivalent to maximum allowable rate 3 L/ft^2/day) from office and graduate housing (daily employee load of ~50 people) of the University of Florida's Gulf Coast Research and Education Center. During 20-month period (May 2012 to December 2013), soil-water samples were collected from the vadose zone using suction cup lysimeters installed at 0.30, 0.60, and 1.05 m depth, and groundwater samples were collected from piezometers installed at 3–3.30 m depth below the drainfield. A complementary 1-year study using smaller drainfields (0.5 m long, 0.9 m wide, 0.9 m high) was conducted to obtain better insights into the vadose zone. A variety of instruments (including multiprobe sensors, suction cup lysimeters, piezometers, tensiometers) were installed for *in situ* soil characterization in vadose zones.

Our results show that microbially mediated N transformations (primarily nitrification) controlled N evolution in drainfield and subsequent movement of N to groundwater. Hydrologic controls (primarily rainfall during wet season, June-September) facilitated rapid transport of N in the soil profile and diluted different N species breakthrough in groundwater. Mean concentration of total P in STE was 12.7±5.6 mg/L, of which 77% of P was present as dissolved reactive P (DRP), with the remainder as other P (particulate inorganic and organic forms). Most of the STE applied DRP was quickly attenuated in the drainfield due to fixation. For example, mean DRP concentrations at 1.05 m below drainfields of drip dispersal and gravel trench were <0.10 mg/L, which further reduced as STE percolated in the soil profile, resulting in <0.05 mg/L mean DRP in groundwater. Concentrations of four pharmaceuticals (sulfamethoxazole, carbamazepine, acetaminophen, and ibuprofen) and three hormones (estrone, 17β-estradiol, and ethinyl estradiol) below vadose zone were 7–14% of total applied acetaminophen, sulfamethoxale, and estrone. Our mass-balance calculations show that all of caffeine, carbamazepine, and ibuprofen were either accumulated and/or bio-transformed in the vadose zone.

Optimizing Monitoring and Remediation Strategies at the Savannah River Site F-Area, Using the Advanced Simulation Capability for Environmental Management (ASCEM)

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The SRS F-Area Seepage Basins, located in the north-central portion of the U.S. Department of Energy (DOE) Savannah River Site (SRS), include three unlined, earthen surface impoundments that received ~7.1 billion liters (1.8 billion gallons) of acidic, low-level radioactive waste solutions. Soil and groundwater in the F-Area are contaminated with a number of constituents, and the groundwater plume extends from the basins to ~600 m downgradient, where it discharges to a stream. The most hazardous contaminants to potential receptors are uranium isotopes, strontium-90, iodine-129, technetium-99, tritium, and nitrate. Remediation activities included capping of the basins, groundwater treatments using a pump-and-treat system, and a hybrid funnel-and-gate with base injections for immobilization of uranium. Monitored Natural Attenuation (MNA) is a desired closure strategy for the site, based on the premise that rainwater will eventually neutralize acidity of contaminated groundwater, stimulating natural immobilization of uranium in the trailing end of the plume. Critical to assessing the *in situ* treatment requirements and MNA over a long time frame is monitoring and predictive understanding of the long-term tritium transport and uranium sorption behavior.

In this study, we developed a three-dimensional model of flow and plume evolution, including engineered barriers, extraction, and injection wells, and key stratigraphic features. We also developed a geochemical reaction network to describe the engineering treatment of base injections. We used newly developed software under the Advanced Simulation Capability for Environmental Management (ASCEM) that includes state-of-the-art numerical methods for simulating complex flow and reactive transport, and toolsets such as uncertainty quantification and parameter estimation. Simulation results are compared with monitoring data, such as pH rebound observed following wellbore-based pH manipulation. The study also includes uncertainty quantification to quantify the uncertainty in future prediction, as well as to identify the key controls for subsurface processes and the most important parameters for accurate predictions. Modeling results can be used to guide monitoring activities and operational decisions, such as when to transition from active remediation to MNA.

Does the Concentration of Ammonical N Fertilizer Affect N_2O Production in Soil, and Why?

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When aiming to develop adequate mitigation strategies for emission of nitrous oxide (N_2O) from soils, an accurate understanding of biochemical N_2O production pathways and their factors in soil is advantageous. Nitrification, nitrifier denitrification, and heterotrophic denitrification are considered as the main pathways of N_2O production, depending on soil conditions such as soil pH, oxygen (O_2) content and substrate. Many researchers have reported that N_2O production increased as substrate concentration increased. However, there is only limited understanding of the mechanism of N_2O production as affected by N concentration. We used two agricultural soils to investigate the effect of ammonium sulfate concentration on the oxygen consumption and pathways of N_2O production under 50% of water-holding-capacity soil moisture. In both soils, oxygen consumption rate and N_2O production rate were increased as ammonium concentration increased.

Theme 6: Defining and Visualizing Complexity Across Scales

Multiscale Visualization of Complex Subsurface Processes

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This talk explores several strategies for how to effectively visualize complex subsurface processes using multiscale visualization techniques within the VisIt visualization framework. VisIt is a turnkey application built to support a host of visualization capabilities and is designed to render at scales ranging from local desktops to high performance computing cluster ecosystems. The visualization methods explored during this talk will illustrate steps on how to construct a compelling visualization that also incorporates geospatial information, well data, highlighting layers, as well as different labeling and annotation strategies to provide a compelling visual result.

To showcase how to apply these steps in a comprehensive way, we highlight VisIt's role within the Advanced Simulation Capability for Environmental Management (ASCEM) project. Specifically, on visualizations developed for the Savannah River F-Area Site and the Hanford Site Deep Vadose Zone, both DOE sites marked for long-term cleanup efforts.

Finally, the talk will also include an overview of several advanced operations within VisIt, such as expressions and querying, which enable users to get the most out of their visualization and analysis.

Remote sensing of belowground variation in trembling aspen forests

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Recognition of the tight linkage between above- and belowground systems can afford important information about soil microbial communities. The chemical traits of forest canopies that are important to soil microbial communities are increasingly measurable via remote sensing platforms. For instance, imaging spectroscopy can provide detailed chemical information about forest canopies by measuring reflectance across a wide range of the electromagnetic spectrum at fine spectral and spatial resolutions. Recent advances in remote sensing indicate that imaging spectroscopy can be used as proxies for important aboveground ecological traits. Here, we demonstrate that imaging spectroscopy can also be used as a proxy for belowground systems. We employed NASA's airborne imaging spectrometer, AVIRIS, to measure both above- and belowground variation in trembling aspen (*Populus tremuloides*) forests.

Across two ecoregions of the continental US, we sampled aboveground aspen genotype and chemistry, and belowground biogeochemistry and microbial communities. While one of our primary goals was to measure variation in aboveground chemistry and aspen genotype, our work also demonstrates that remote sensing can provide information regarding belowground systems. Variation in AVIRIS imagery was well correlated with variation in belowground enzyme activities, C, N, and extractable NH_4+ and NO_3-. Moreover, remotely-sensed imagery was better correlated with belowground functional responses than were commonly measured plant chemistries (C, N, tannin, lignin). Ongoing work indicates that in addition to serving as a proxy for microbial functional responses, AVIRIS imagery can also provide taxonomic information as suggested by next generation sequence analysis of soil bacterial and fungal communities. While we cannot correlate specific taxa with specific AVIRIS spectra at this point, imaging spectroscopy is related to simple belowground diversity indexes generated from Illumina MiSeq runs. These results suggest that remote sensing technologies can be used to describe the fine-scale variation in belowground systems across large spatial scales that is otherwise not feasible via traditional field collection methods.

Measuring and Scaling Dynamic Soil Properties in Soil Survey

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Traditional soil survey products deliver information about soil properties without taking into account current land-use or management systems. Soil surveys vary in the scale of information they provide on spatial, taxonomic, and property-specific scales. The order and purpose of a given soil survey impacts spatial scale and the design soil mapping units. Map-unit design includes decisions about the types of map units (consociations, associations, or complexes) used as well as the arrangement and composition of those map units. The individual map-unit components have their own scales—how finely are taxonomic classes defined, or how many different slope classes should be recognized. In the NCSS, soil property information is then attributed to map-unit components using available data and expert knowledge. Decisions about the inclusion of data (is it part of the central concept?) and rules-of-thumb about appropriate property classes impact the values (low–representative value (rv)–high) populated in available databases such as SSURGO. Currently, the NCSS uses the Soil Change Guide to organize the collection of use-dependent properties under the name Dynamic Soil Properties (DSPs). In this conception, additional decisions impact the spatial and conceptual scales of the data. For current DSP projects, on one soil component, two or more conditions are selected that represent the "best" and most common management systems in common land uses. The range of data collected depends on how tightly the soil components selected represent the central concept, and how the comparison of systems was constructed. Critical questions remain about how this information is extrapolated across multiple scales and conditions. Incorporating soil-landscape-ecosystem systems into corporate hierarchies will allow us to apply information from DSP projects to similar soils. Further work is needed to link and expand ecosystems, land use/cover types, and management systems.

Soil Landscape Systems: A Scalar Framework for Modeling Soil Processes and Properties

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A catena is a recurring landscape array of soils from an upland divide to a stream or topographic low. A Soil Landscape System is one or more catenas that dominate an area based on parent materials, geomorphology, local relief, and hydrologic connectivity within a climate regime. The soil landscape is the dominant scalar control on soil processes and properties. Process and spatial models that are data driven have greater utility and scalar reliability when stratified by the Soil Landscape System. The soil landscape framework shifts emphasis away from pedon-centric data and purely statistical modeling. Soil Landscape Systems (a) provide a critical link between soil point data and ecosystem processes at multiple scales, (b) represent a quantifiable model that explains soil patterns and processes that underpin spatial models, (c) integrate hydropedology to explain soil distribution and function, and (d) provide a conceptual model to communicate soil knowledge across scientific disciplines and to general audiences.

Theme 7: Moving Forward – Research Coordination, Building the Ecosystem

Data Coordination for Multi-Scale Complex Systems Analysis

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Soil data are important in developing an understanding of hydrological, biological, geochemical, and other processes, as well as the interactions between these processes. We have been developing data management systems to support watershed, regional, and global analyses. In this presentation I will discuss our approach to soils data management in the AmeriFlux, Sustainable Systems SFA, FLUXNET, and International Soil Carbon Network data management systems.

On the Need to Establish an International Soil Modeling Consortium

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Soil is one of the most critical life-supporting compartments of the biosphere. Soil provides numerous ecosystem services, such as a habitat for biodiversity, water, and nutrients, as well as producing food, feed, fiber, and energy. To feed the rapidly growing world population in 2050, agricultural food production must be doubled using the same land resources footprint. At the same time, soil resources are threatened due to improper management and climate change.

Soil is not only essential for establishing a sustainable bio-economy, but also plays a key role in a broad range of societal challenges including (1) climate change mitigation and adaptation, (2) land-use change, (3) water resource protection, (4) biotechnology for human health, (5) biodiversity and ecological sustainability, and (6) combating desertification. Soils regulate and support water, mass and energy fluxes between the land surface, the vegetation, the atmosphere, and the deep subsurface and control storage and release of organic matter affecting climate regulation and biogeochemical cycles. Despite the many important functions of soil, however, many fundamental knowledge gaps remain regarding the role of soil biota and biodiversity on ecosystem services, the structure and dynamics of soil communities, the interplay between hydrologic and biotic processes, the quantification of soil biogeochemical processes and soil structural processes, the resilience and recovery of soils from stress, as well as the prediction of soil development and the evolution of soils in the landscape— to name a few.

Soil models have long played an important role in quantifying and predicting soil processes and related ecosystem services. However, a new generation of soil models based on a whole systems approach—comprising all physical, mechanical, chemical, and biological processes—is now required to address these critical knowledge gaps and thus contribute to the preservation of ecosystem services, improve our understanding of climate-change–feedback processes, bridge basic soil science research and management, and facilitate the communication between science and society . To meet these challenges, an international community effort is required, similar to initiatives in systems biology, hydrology, and climate and crop research.

We therefore propose to establish an international soil modeling consortium with the aims of 1) bringing together leading experts in modeling soil processes within all major soil disciplines, (2) addressing major scientific gaps in describing key processes and their long-term impacts with respect to the different functions and ecosystem services provided by soil, (3) intercomparing soil-model performance based on standardized and harmonized data sets, (4) identifying interactions with other relevant platforms related to common data formats, protocols, and ontologies, (5) developing new approaches to inverse modelling, calibration, and validation of soil models, 6) integrating soil modeling expertise and state of the art knowledge on soil processes in climate, land surface, ecological, crop, and contaminant models, and (7) linking process models with new observations, measurements, and data evaluation technologies for mapping and characterizing soil properties across scales. Our consortium will bring together modelers and experimental soil scientists at the forefront of new technologies and approaches to characterize soils. By addressing these aims, the consortium will contribute to improving the role of soil modeling as a knowledge dissemination instrument in addressing key global issues and stimulating the development of translational research activities. This presentation will provide a compelling case for this much-needed effort, with a focus on tangible benefits to the scientific and food-security communities.