2021 AAAS Annual Meeting, February 8-11, 2021 https://meetings.aaas.org/

Accepted Special Session: **Coupled Experimental and Multiscale** Modeling Study of the Environmental Microbiome

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Session Description: Microbial communities determine the biogeochemical cycles of the earth's soil, oceans and the atmosphere, and perform ecosystem functions that impact plants, animals and humans. Yet our ability to predict and manage the function of these highly complex. dynamically changing communities is limited. The complexity and dynamics of community behavior presents challenges that are difficult to address with experimental observation alone. With microbiology emerging as a quantitative science, strong opportunities exist for integrating theoretical insights and experimental approaches. Indeed, study of fundamental principles and mechanisms with mathematical models has a novel discovery potential for complex biological and ecological systems that is underutilized and unrecognized. This Special Session will provide an overview of coupling experimental studies and mathematical modeling of interactions within natural ecosystems, emphasizing that a critical aspect in the development of mathematical models is the need to address appropriate and multiple scales to understand the emergent behavior of the microbial community that is encoded in the data. While these scales can be addressed using population dynamics, stochastic dynamical systems or metabolic network models using both systems of ODEs and PDEs, in order to employ theoretical models fully and successfully it is vital to implement an interdisciplinary view during the conceptual design of the experiments and in the post-experiment interpretation of the data and phenomena.

Relevance to Theme or Special Relevance to the Audience: The focus of this session on understanding complexity, adaptation and stability in environmental microbial communities is directly related to the study of dynamical ecosystems and microbiomes to promote sustainable change. Approaches to be discussed are rooted in several fields represented within AAAS, including mathematics, microbial ecology, systems biology, physics, statistics and computational science. The session will present research that has successfully crossed these disciplines as well as the cultural boundaries separating them. The scientists engaged in the work have learned to effectively communicate across disciplines, which will make their presentations accessible and of interest to a diverse audience.

Section Affiliation: Mathematics (A), Biology (B)

Keywords: plant microbiome, ecosystems, multiscale mathematical modeling, computational biology, data analysis

Speaker: Jenny Kao-Kniffin, Associate Professor, School of Integrative Plant Science, Cornell University, USA

Title: Assembly of highly connected microbiomes that modify plant host traits

Abstract: Directed evolution provides a system to study rapid changes in microbial interactions associated with a specific host trait. We share results from two separate experiments involving microbiome assembly through selective pressure on plant phenotypes—flowering time in *Arabidopsis thaliana* and plant productivity in *Brassica rapa*. Microbiomes associated with a specific plant trait were continuously patched across nine to ten successive plantings by collecting soil from the root zone of plants exhibiting the greatest modifications to the targeted trait. In both studies, similar properties of the microbiome emerged. The density of associations across microbial taxa were enhanced, with more edges and connectivity, in plant systems of greater productivity. Multiple models were used to characterize the interactions across taxa. As theoretical systems involving microbial adaptation to a host or ecosystem trait becomes more widely adopted, it may become feasible to identify microbial group behaviors and composition that are closely linked to host function.

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Speaker: Ross Carlson, Professor, Department of Chemical and Biological Engineering, Thermal Biology Institute, Center for Biofilm Engineering, Montana State University, Bozeman, Montana, United States of America, USA

Title: Multiscale analysis of autotroph-heterotroph interactions in a high-temperature, ironoxidizing microbial community

Abstract: Microbial interactions can result in emergent properties, such as enhanced productivity, stability, and robustness. These emergent properties are of great interest to scientific fields ranging from the study of global nutrient cycling including greenhouse gases to biofuels synthesis. Acidic (pH 2 – 4), high-temperature (> 65 $^{\circ}$ C) springs in Yellowstone National Park are excellent model systems for studying microbial populations and their interactions due to their relative simplicity. This study integrated data collected in situ from an iron-oxidizing microbial community with in silico calculations across length-scales encompassing enzymatic activity, cellular metabolism, community interactions, and ecosystem biogeochemistry. Experimental omics data were used to reconstruct in silico metabolisms of an important CO₂fixing, autotroph and a heterotroph from the springs. The metabolic reconstructions were analyzed using standard and hybrid, applications of elementary flux mode and flux balance analyses to predict cellular- and community-level activities. In situ geochemical analyses, including oxygen concentrations, iron-oxide deposition rates, stable carbon isotope patterns, and community biomass concentrations, were combined with the in silico models to predict autotroph-heterotroph interactions and to quantify the functional limits of the interactions. Integration of metabolic modeling with in situ measurements demonstrated that the communities operated at their maximum total community growth rate, as opposed to the maximum net community growth rate, consistent with the ecological theory of maximum power principle. Integration of multiscale data with ecological theory provides a basis for predicting autotrophheterotroph interactions and community-level organization.

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Speaker: Orkun Soyer, Professor, School of Life Sciences, Co-Director, Warwick Integrative Synthetic Biology Centre, University of Warwick, UK

Title: Temporal and spatial organization in microbial communities

Abstract: Microbial communities are complex dynamic systems. In addition, communities can form spatial organization as seen in the case of biofilms, granules, or mats. The understanding of temporal dynamics and its relation to function can be studied through temporal sampling of natural communities with relatively well-defined function. I will summarize findings from a 1 year-long study we have devised to this end, focusing on industrial anaerobic digestion reactors. Our findings show that temporal community dynamics across reactors is distinct and show correlations with functional output parameters. Furthermore, temporal dynamics allows identification of within community interactions and provide insights into functional roles of individual organisms. In summary, the talk will highlight the importance and value of temporal study of communities' function.

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