Prediction of Spatial Assemblies in Soil Microbiomes Governed by Interspecies Interactions and Environmental Gradients

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Project Goals: PNNL's Phenotypic Response of Soil Microorganisms SFA aims to achieve a systems-level understanding of the soil microbiome's phenotypic response to changing moisture. We perform multi-scale examinations of molecular and ecological interactions occurring within and between members of microbial consortia during organic carbon decomposition, using chitin as a model compound. Integrated experiments are designed to confront spatial challenges and inter-kingdom interactions among bacteria, fungi viruses and plants that regulate community functions. These data are used to parametrize individual- and population-based models for predicting interspecies and inter-kingdom interactions. Predictions are tested in lab and field experiments to reveal individual and community microbial phenotypes. Data is captured and shared through an optimized data management pipeline. Knowledge gained will provide fundamental understanding of how soil microbes interact to decompose organic carbon and enable prediction of how biochemical reaction networks shift in response to changing moisture regimes.

Heterogeneous micro-patches in soil lead to spatial distributions in microbial communities. The formation of spatial patterns is not random but governed by numerous biotic and abiotic factors, including metabolic and chemotactic traits of individual members, interspecies interactions, and environmental factors. It is critical to understand how environmental constraints control the formation of specific spatial patterns through the modification of interspecies spatial interactions. However, elucidating key biological and environmental parameters governing specific spatial patterns of interacting species remains challenging, partly due to the lack of reliable computational and instrumental tools that can be effectively used for this purpose. Toward filling this gap, here we present coordinated modeling and experimental approaches for predicting and visualizing spatial formation of microbial assemblies.

First, we developed an agent-based model to predict spatiotemporal evolution of interacting species at the microscale (μm to mm)[1]. The simulated spatial patterns obtained from the agent-based model were subsequently used to train deep learning models to infer microbial interactions. The resulting machine learning model accurately inferred the spatial variation in microbial interactions in heterogeneous environments as demonstrated through a case study of *Pseudomonas fluorescens* and *Escherichia coli*. This co-culture developed context-dependent interactions when treated with polymeric chitin or N-acetylglucosamine (NAG, the hydrolysis product of chitin) because *P. fluorescens* can use both substrates for growth, while *E. coli* lacks the ability to degrade chitin.

To extend the modeling scope of spatial interactions to larger scales (up to cm), we developed a multi-component, multi-species reaction-diffusion model. Unlike agent-based models where microbial cells are treated as discrete particles, reaction-diffusion models provide a continuous description of the distribution of microorganisms as well as chemical nutrients in a multi-dimensional space. We formulated this model to simulate spatial interactions and assemblies of multiple isolates derived from our Model Soil Consortia[2]. Key variables we accounted for this purpose included chemotactic motion of microorganisms, spatial gradients of nutrients (such as chitin or NAG), and moisture levels. We parameterized basic metabolic and chemotactic features of species based on (1) genome-scale metabolic network models of isolates built using the DOE's KBase pipeline[3], and (2) microbial growth data using microchip experiments.

Predicted spatial interactions and microbial assemblies were also experimentally validated using visualization techniques. As a proof-of-concept study, we developed a dynamic model of a *Cellvibrio japonicus* and *E. coli* consortium to simulate the interactions among degraders (chitin-degrading *C. japonicus*), lazy friends (non-chitin-degrading *C. japonicus*), and cheaters (*E. coli*) in the homogeneous environment. In addition we tested and optimized conditions for labeling chitinase enzymes *in vivo* with a chitinase activity-based probe (chitotriose-ABP). Beyond predicting the optimal proportion of degraders in the presence and absence of cheaters, this model enabled the evaluation of the ecological benefit of spatial assemblies of soil microorganisms in promoting community function.

New developments of modeling and visualization methods in this work provide an improved capability of (1) predicting the evolution of soil microorganisms in spatially constrained environments, and (2) inferring interspecies interactions from the resulting image data. Incorporation of genome-scale metabolic networks into agent-based and reaction-diffusion models for more mechanistic simulations are currently in progress.

References:

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