

THE EVOLUTION OF METABOLIC COMMUNITIES: COMPUTATIONAL MODELS AND EMPIRICAL RESULTS. H. B. Smith^{1*}, H. Kim² and J. Raymond¹, S. I. Walker^{1,2,3}, ¹School of Earth and Space Exploration, Arizona State University, Tempe, AZ, USA, ²Beyond Center for Fundamental Concepts in Science, Arizona State University, Tempe, AZ, USA, ³Blue Marble Space Institute of Science, Seattle, WA USA.
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Introduction: Biological evolution is typically depicted as a passive process, whereby life is shaped by its environment. However, in reality life is strongly coupled to its planetary environment: evolution is a complex, dynamical process with feedback between environment and organisms [1]. Thus, environments reflect and record not just geochemical processes, but the interaction of biology and geochemistry [2,3]. This interplay between life and planetary processes is important on our own planet, where it has shaped the co-evolution of life and Earth [4]—and should be equally important for extraterrestrial ecosystems. This requires deriving insights into universal principles that might underlie biological organization within a planetary context.

One feature that holds promise to potentially be a universal attribute of biology is network architecture. Biological networks studied across a range of length and timescales—such as neural networks, gene regulatory networks, or cell signaling networks [5-7]—have some features in common, including scaling laws for the distribution of connectivity of network nodes. Organismal metabolic networks have also been shown to share this feature [8]. Metabolic networks are particularly relevant to the question of the co-evolution of life and environment as they provide the most direct information about the mechanisms and processes by which organisms interact with their geochemical environment to transform chemical species and evolve [9].



Figure 1. Metabolic networks inferred from Yellowstone National Park (YNP) metagenomic data. Networks consist of data from 26 metagenomes throughout diverse hot spring communities in YNP. Left: Sampled phototrophic communities. Right: Sampled chemotrophic communities. Center: Both communities combined. Nodes shared by both communities in light blue. Nodes exclusive to chemotrophic communities in dark blue. Nodes exclusive to phototrophic communities in red.

Empirical Analysis: We are studying the metabolic networks of microbial communities in hot spring ecosystems across a range of pH, temperature, and elemental abundance (Figure 1) [10]. Precursory network analysis of these communities has revealed that

they are scale free, like a scaled version of individual organismal metabolic networks. Analyses of reactions catalyzed within communities have also revealed that across diverse sample sites, communities have the same distribution of reactions catalyzed vs. enzymes doing catalysis. Whether these patterns are a result of selection at the individual or communal level, and why the same pattern would emerge across different environments has yet to be determined

Computational Model: We are developing a comprehensive computational model to study the evolution of metabolic communities in an environmental context. Our model consists of a spatial grid containing organisms—defined by their enzyme repertoire—and metabolites—defined by a binary string of length m . The system allows for 2^m metabolites, which undergo reactions (transformations) when catalyzed by an enzyme. The propensity for any given reaction is proportional to the concentration of the two reactants, the concentration of any catalyzing enzymes, and each enzyme's reaction specific rate constant. Using the Gillespie Algorithm, a variant of the Kinetic Monte-Carlo algorithm [11], a reaction is simulated every time step, chosen by a probability distribution weighted by reaction propensities. After each time step, propensities are updated to reflect changes to the system. Reactions provide energy to their organisms, which then use this energy to reproduce once they reach an energy threshold. Organisms can also die when they consume too much energy without gaining energy from metabolic transformations.

Preliminary results of our computational model and the insights they provide into the empirically observed network structure of metabolic communities will be reported.

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