Molecular level *in silico* analysis of mass and energy flows in microbial communities

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Motivation:

Complex microbial communities drive the Earth's biogeochemical cycles. In spite of their importance, the biochemical interactions within these communities are not yet well understood, nor are many *in silico* methodologies available for studying them.

Background:

Three methods were developed for the application of stoichiometry-based network analysis approaches to the study of mass and energy flows in microbial communities. Each has distinct advantages and disadvantages suitable for analyzing systems with different degrees of complexity and *a priori* knowledge. These approaches were tested and compared using data from the thermophilic, phototrophic mat communities from Octopus and Mushroom Springs in Yellowstone National Park (USA). The models were based on three distinct microbial guilds: oxygenic phototrophs, filamentous anoxygenic phototrophs (FAP), and sulfate-reducing bacteria(SRB). Two phases, day and night, were modeled to account for differences in the mass and energy sources and the routes available for their exchange.

The *in silico* models were used to explore fundamental questions in ecology including the prediction of and explanation for measured relative abundances of primary producers in the mat, theoretical tradeoffs between overall productivity and the generation of toxic by-products, and the relative robustness of various guild interactions.

The three modeling approaches represent a flexible toolbox for creating cellular metabolic networks to study microbial communities on scales ranging from cells to ecosystems.