

## **A Trait Based Dynamic Energy Budget Approach to Explore Emergent Microalgal Community Structure**

Yiwei Cheng<sup>1\*</sup> (yiweicheng@lbl.gov), Ulas Karaoz<sup>1</sup>, Nicholas J. Bouskill<sup>1</sup>, **Jennifer Pett-Ridge<sup>2</sup>**, **Xavier Mayali<sup>2</sup>** and **Eoin L. Brodie<sup>1</sup>**

<sup>1</sup>Lawrence Berkeley National Laboratory, Berkeley, CA; <sup>2</sup>Lawrence Livermore National Laboratory, Livermore, CA.

**Project Goals: The LLNL Biofuels SFA seeks to support robust and sustainable microalgae fuel production through a systems biology understanding of algal-bacterial interactions. A goal of the SFA is the predictive modeling of complex microbial communities in open pond microalgae dominated ecosystems. Towards achieving that goal, a microbial model capable of representing key mechanistic properties that determine fitness of microbial populations in dynamic systems, and with robust mechanistic representation of intra-cellular resource allocations is key to improve realism of the simulated microbial community dynamics. Mechanistic models also have the potential to enhance fundamental understanding of the underlying ecological principles of algal-bacterial interactions. Through integration with empirical knowledge, mechanistic models also provide a more robust platform valid for wider range of scenarios.**

Research has been underway for decades to realize the full potential of algal biofuels at the commercial scale, however, monoculture algal ponds are typically threatened by collapse due to microalgal grazing and parasite invasions. Recently, it has been proposed that functionally diverse microalgal-bacterial communities can achieve higher biomass and/or lipid yields, and are more stable (less susceptible to invasion) than monocultures. Similar positive diversity-productivity relationships have been observed in a wide range of ecosystem studies, but the purposeful maintenance of a diverse microbiome is less common in managed systems.

We have developed a trait based dynamic energy budget model to explore emergent microalgal community structure under various environmental (e.g. light, temperature, nutrient availability) conditions. We initially reduce the complex algal community into functional groups (guilds). Each microbial guild (algae or bacteria) is characterized by distinct combination of physiological traits (e.g. nutrient requirement, growth rate, substrate affinity, lipid production) constrained by biochemical trade-offs. These trait values can be derived from literature or genomic data. Metabolism of the algae and the bacterial species (symbiotic or non-symbiotic) are described within a dynamic energy budget framework. Currently, the trait values follow those from the literature and will be refined based on the results from experimentation and flux balance and multi-objective flux modeling, represent initially *Phaeodactylum tricornutum*, *Chlamydomonas reinhardtii* and *Nannochloropsis salina* as model algal species. Our model offers a mechanistic framework to predict the optimal microalgal community assemblage towards achieving higher productivity and resistance to invasion under prevailing environmental conditions.

In our initial investigation into the mathematical representation of uptake kinetics, we compared simulation results of two uptake formulations: equilibrium chemistry approximation kinetics (ECA) and Michaelis-Menten (MM) kinetics. The ECA formulation has previously been shown to be more accurate in certain cases such as a single microbe utilizing multiple substrates and multiple microbes utilizing multiple substrates. In this work, initial simulation results showed that MM kinetics tend to overestimate algal biomass when compared to ECA kinetics.

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