Los Alamos
NATIONAL LABORATORY

MetConSIN

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MetConSIN

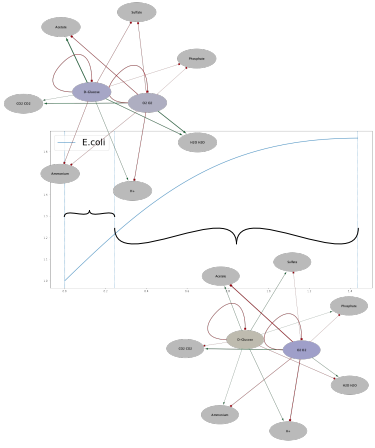
Concept:

- Genome-scale models and constraint based methods are commonly used and allow us to use knowledge of microbial genome sequences to predict metabolic behavior.
- This modeling paradigm implies a dynamical system that couples optimization with differential equations, and is very difficult to simulate and analyze.
  - Naively, optimization must be done at every time-step.
  - Really, optimization is only required at a (relatively) sparse set of time-points.
- This dynamical system can be understood as a sequence of simpler dynamical systems which model species-metabolite interaction networks.

Planned Implementation:

- Use metagenomic sequencing of environmental samples to build genome scale models of microbial community members.
- Simulate community genome (metagenome) scale dynamics of metabolism.
- Identify time intervals of constant network topology & corresponding networks.
- Identify impactful transitions in network topology.
- Develop simplified & tractable predictive modeling for design & engineering by leveraging the “sequence of networks” structure of the microbial community.

MetConSIN



During simulated growth of *E. coli*, we observe two distinct networks of interactions between metabolites (as mediated by *E. coli*).

Idea

Simulating a microbiome (microbes & external metabolites) using genome scale metabolic models provides a dynamically changing network of interactions.

Using GEMs constructed from metagenomic data, MetConSIN will allow us to

- Understand the interactions of microbes & metabolites in a microbiome.
- Predict & manipulate microbial community composition.
- Predict & manipulate microbiome metabolite production.