Simulating Dead-End State Distributions for Microbial Metabolism

"Microbial ecology ... and other rabbit holes"

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Background

- Microbial metabolic chemistry can be represented using the following equation:

$$\frac{d\boldsymbol{C}}{dt} = \mathbb{S} \cdot \boldsymbol{H} \qquad \textbf{(Eq. 1)}$$

$\boldsymbol{C}_m$ – concentration of metabolite m

$\mathbb{S}_{mn}$ - stoichiometric coefficient of metabolite m in reaction n

$\boldsymbol{H}_n$ - kinetic rate of metabolic reaction n

Dead-End State: a set of metabolite concentrations that makes all reactions energetically unfavorable.

$$\boldsymbol{C}^* \text{ such that } \Delta\boldsymbol{G}_n \geq 0 \text{ for } 1 \leq n \leq N \qquad \textbf{(Eq. 2)}$$

$\boldsymbol{C}^*$ – a dead-end state of **Eq. 1**

$\Delta\boldsymbol{G}_n$ – Gibbs Free Energy yield of reaction n

N – total number of chemical reactions

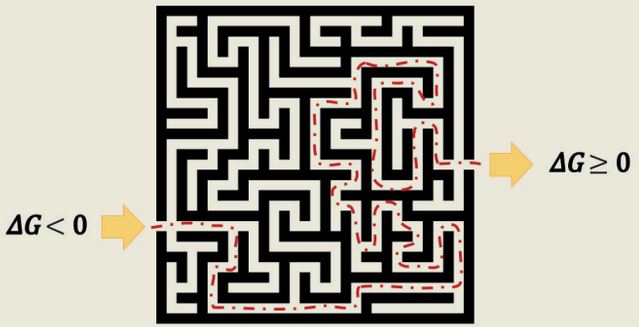

Figure 1: Finding a dead-end state for **Eq. 1** is analogous to finding an exit point through a complex energetic maze.

Solving The Maze: A Computer-Based Approach

- **Central Question**: what can these dead-end states tell us about the ecosystem being modelled by **Eq. 1**?

Our Approach:

1. Run *a lot* of random-walk simulations
2. View graph of possible outcomes

"Throwing the Darts"

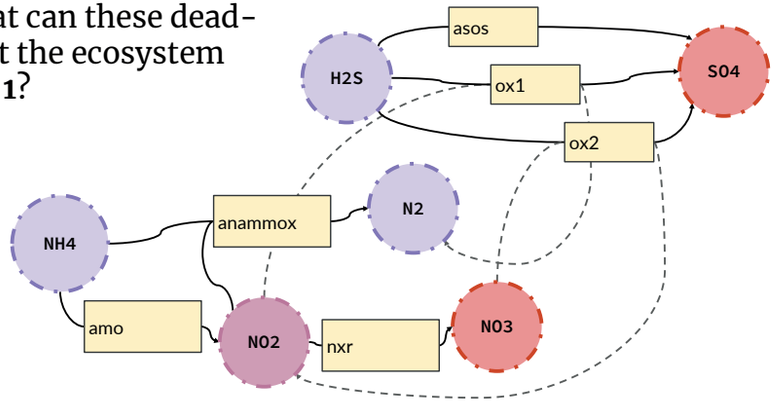

Figure 2: A reaction-centric model consisting of 6 metabolites and 6 chemical reactions.

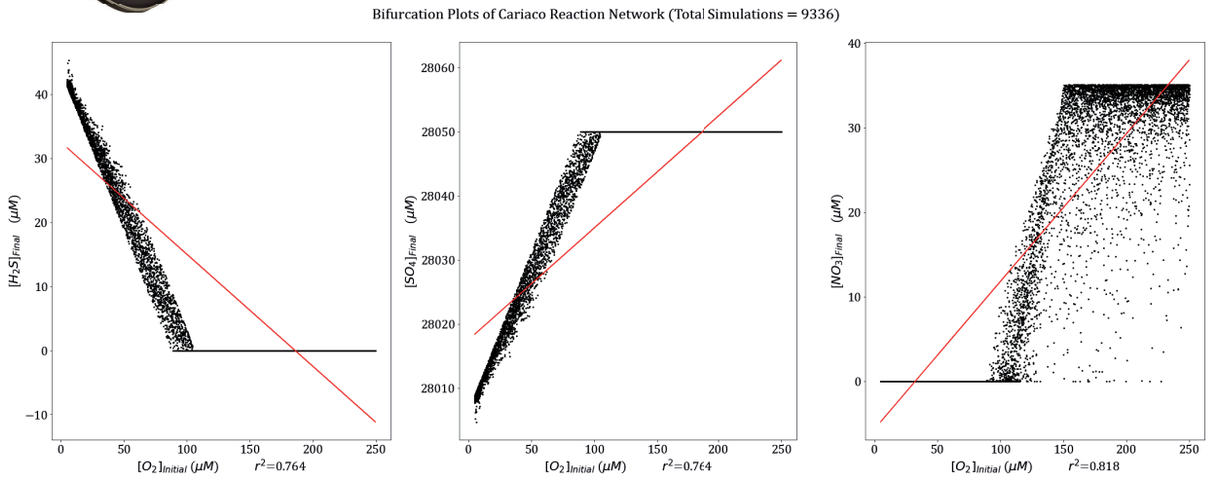

Figure 3: Bifurcation diagram of possible end states for the model presented in **Figure 2.** The end-states were plotted with respect to varying initial oxygen (O_2) concentrations.

Primary References:

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