

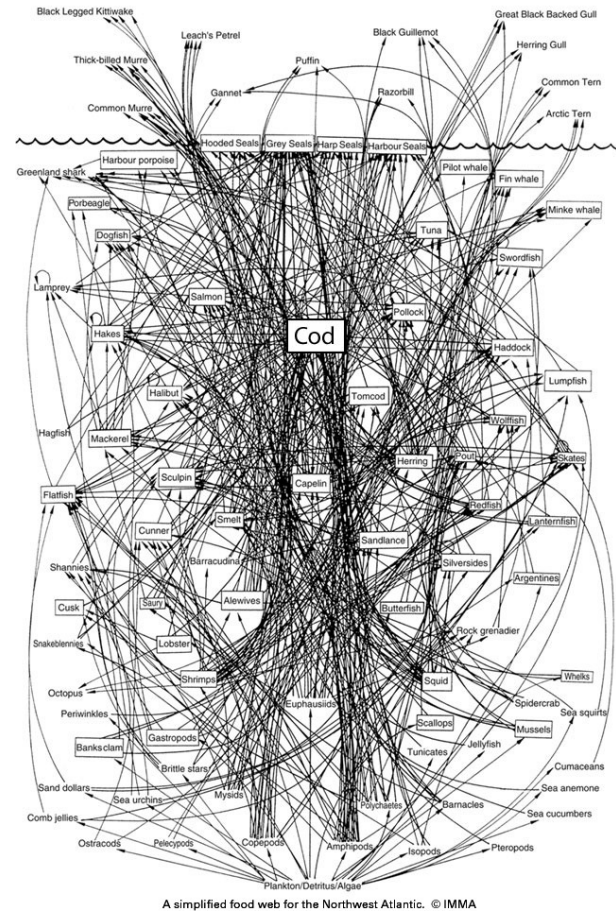
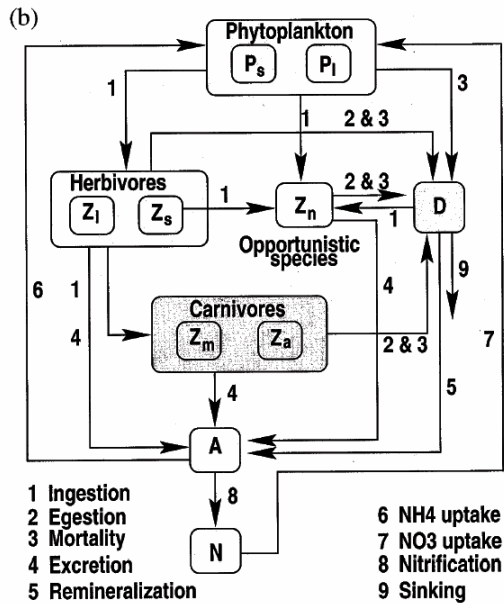
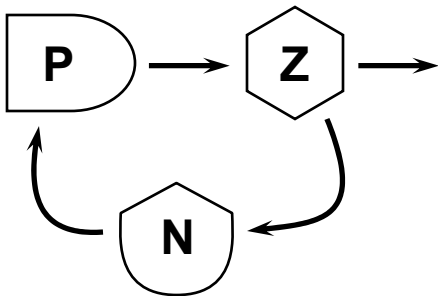
# Can Dynamic Trophic Structures Be Captured in Structurally Fixed Models?

*Joe Vallino*

MBL

Ocean Carbon and Biogeochemistry Workshop  
Woods Hole Oceanographic Institution  
July 23-26, 2007

# Real Food Webs vs. Modeled

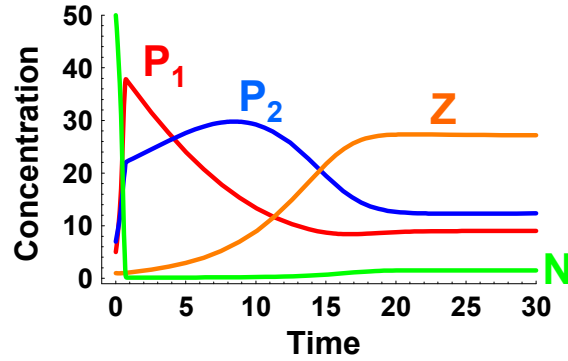
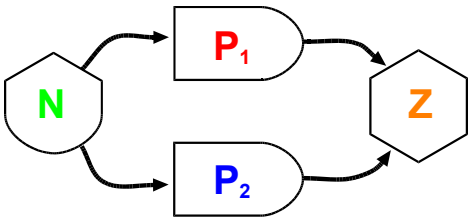


## Main difficulties:

- Compartment aggregation introduces errors.
- Models do not capture change in community composition

# Model Aggregation Errors

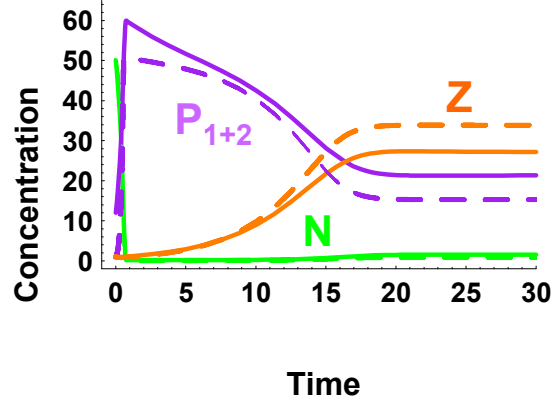
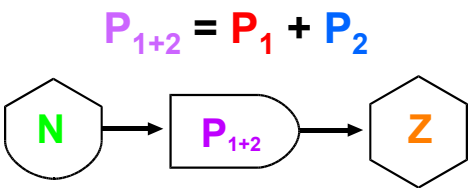
## True Model



## True parameter values

	$V^M$	$K_s$	$P(0)$
$P_1$	4	5	5
$P_2$	2	1	7

## Approx. Model



## Estimated aggregated parameter values

	$V^M$	$K_s$	$P(0)$
$P_{1+2}$	8.2	3.2	1

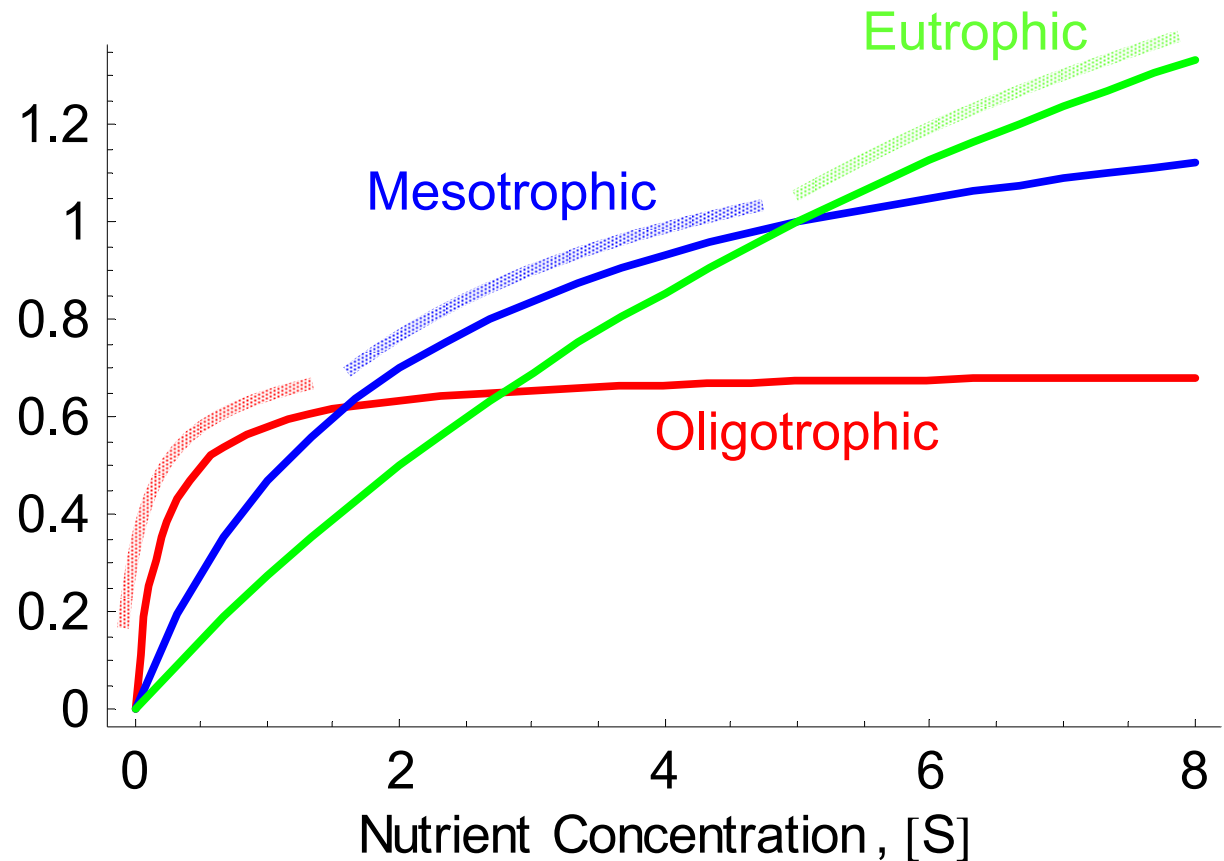
## Main Points

- Models with fewer state variables can not capture true system.
- Parameter values can be very different than expectations.
  - Model must be fit to whole system observations.

# Kinetics and Community Dynamics

Growth kinetics are dependent on the organisms present, which in turn are dependent on environmental resource availability.

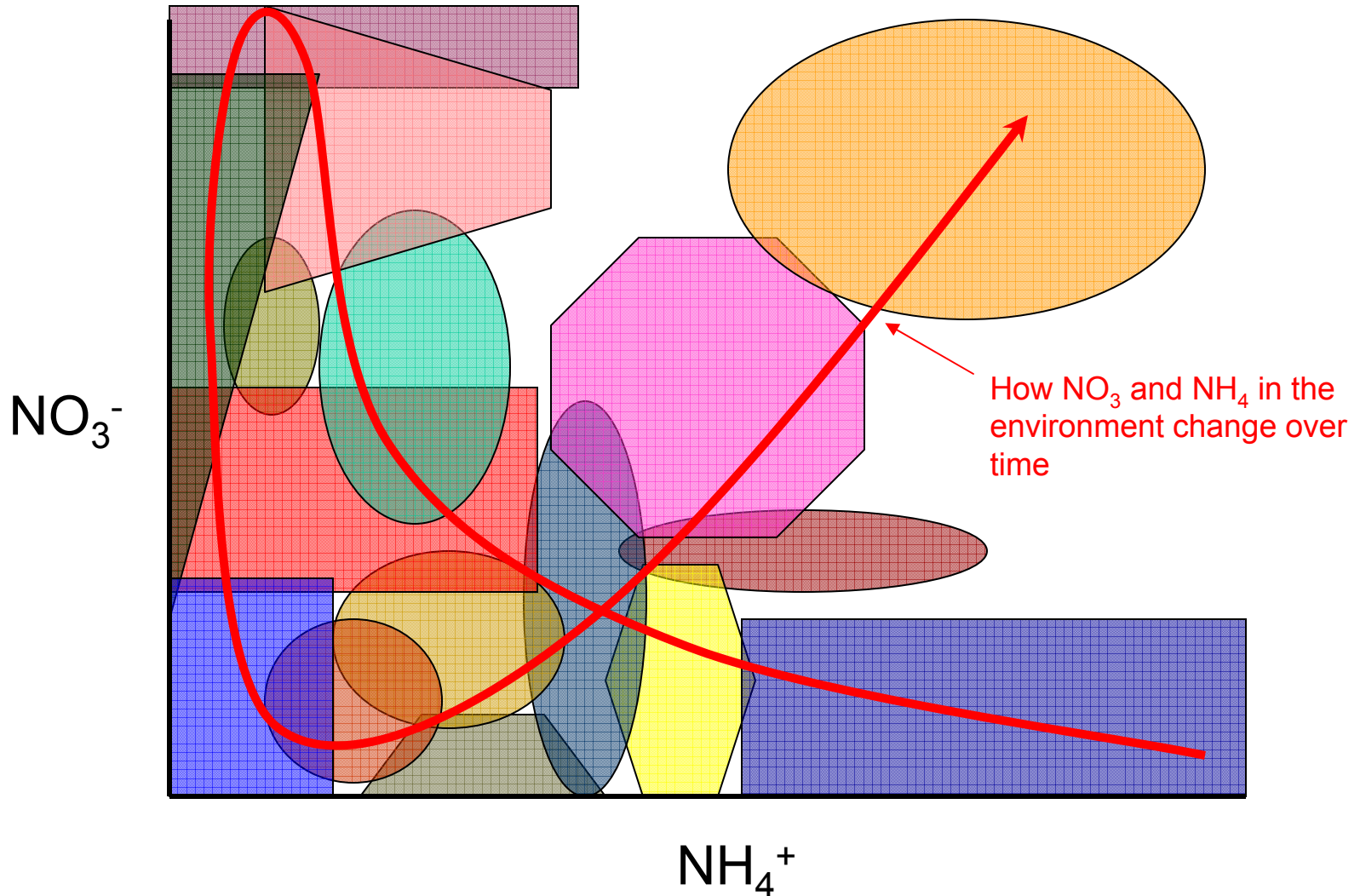
$$V = \frac{V^{Max} [S]}{[S] + K_M}$$



**Model Parameters are Not constants!**

# Community Composition Tracks Environment

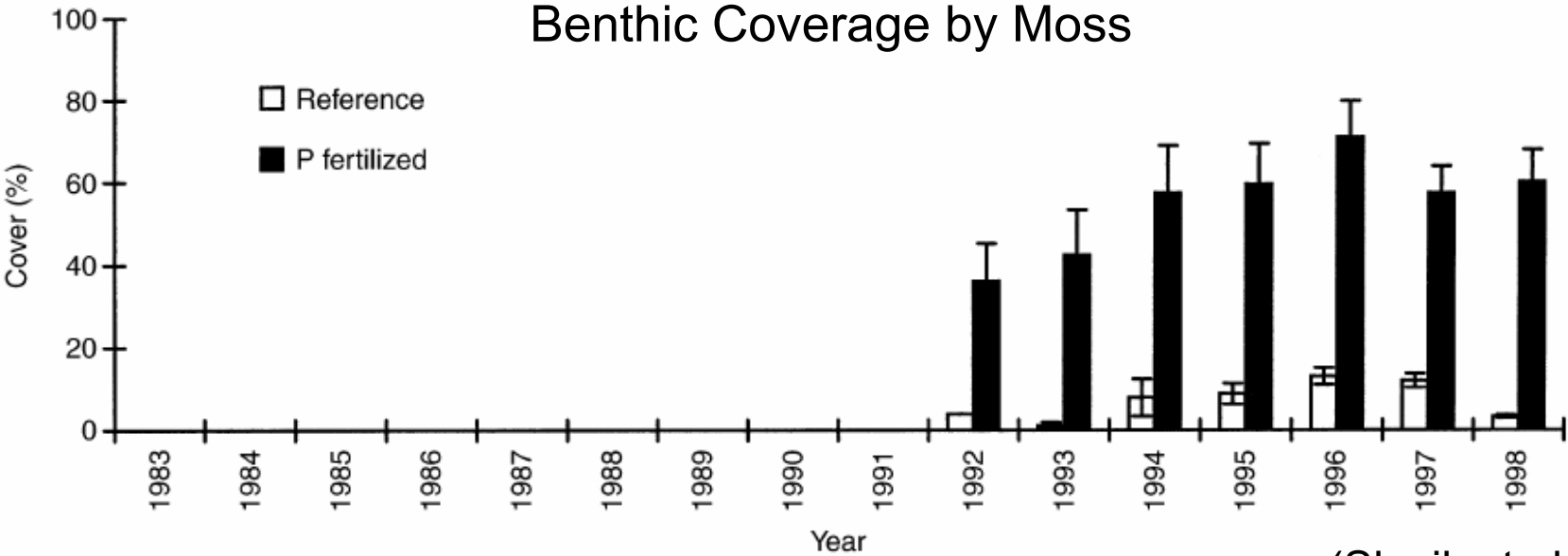
Polygons represent organisms whose growth is optimal for specific conditions



# Example of Community Shift

Change in community structure from long-term fertilization (P) of Arctic stream (Kuparuk River).

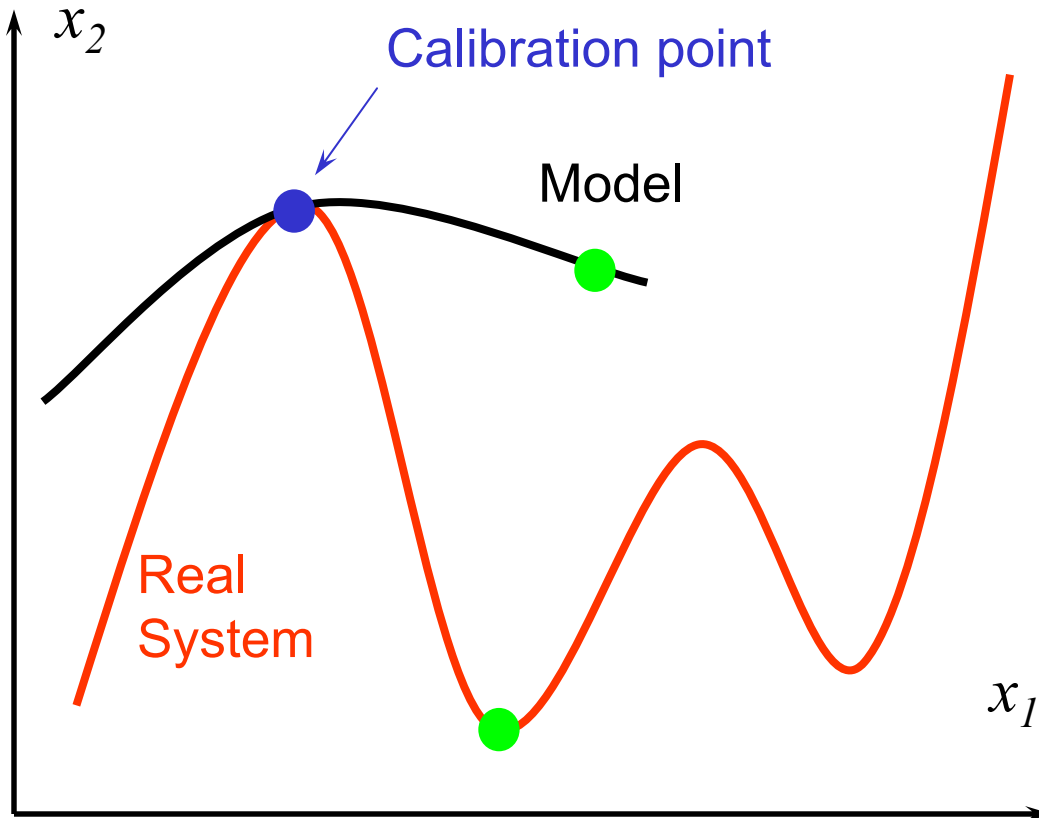
Moss “carpet” forms after 9 years of treatment.



(Slavik et al. 2004)

# Problem with Fixed Model Structure

Since model structure can not adapt to changing community, model extrapolation is poor

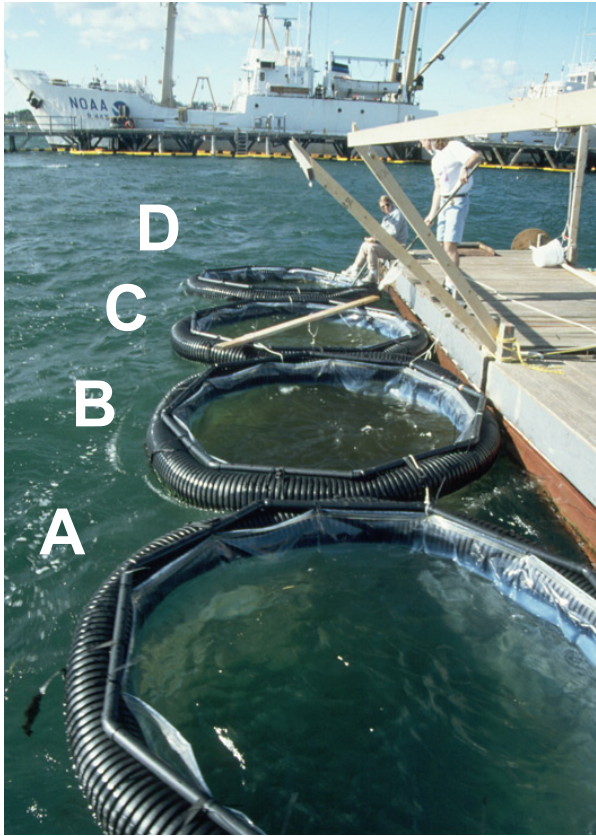




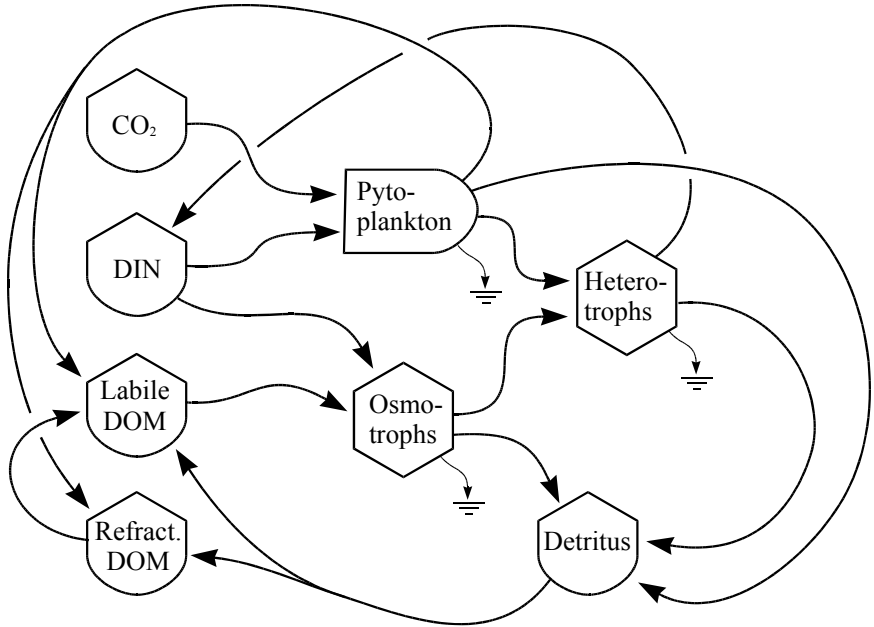
# Mesocosm Experiment Example

## Treatments:

- Control: Bag A
- Organic Matter: Bag B
- Daily Nutrients: Bag C
- DOM + Nutrients: Bag D



## Trophic Model



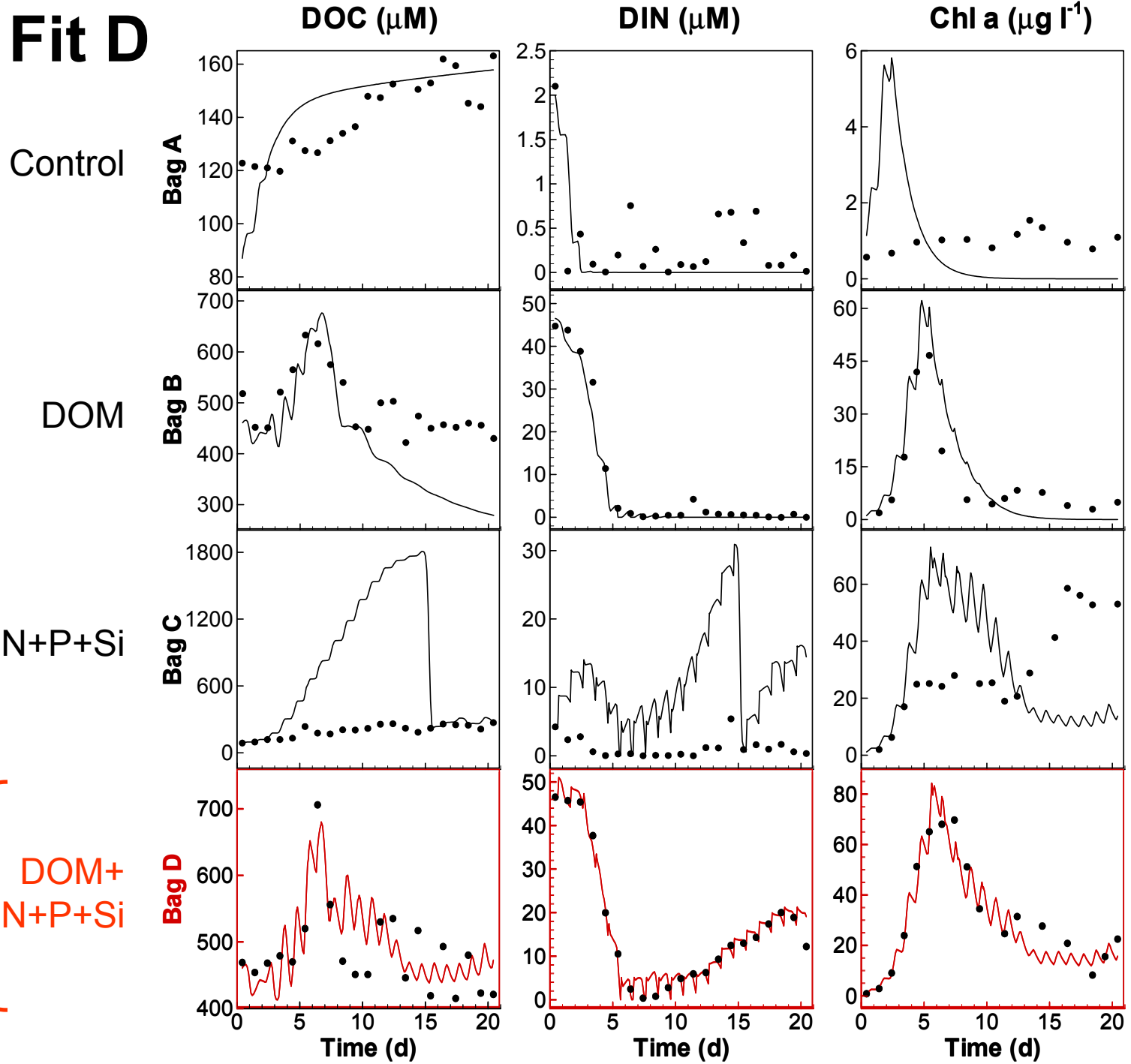
**State Variables: 10**

**Parameters: 39**

- 29 Kinetic
- 10 Initial cond.



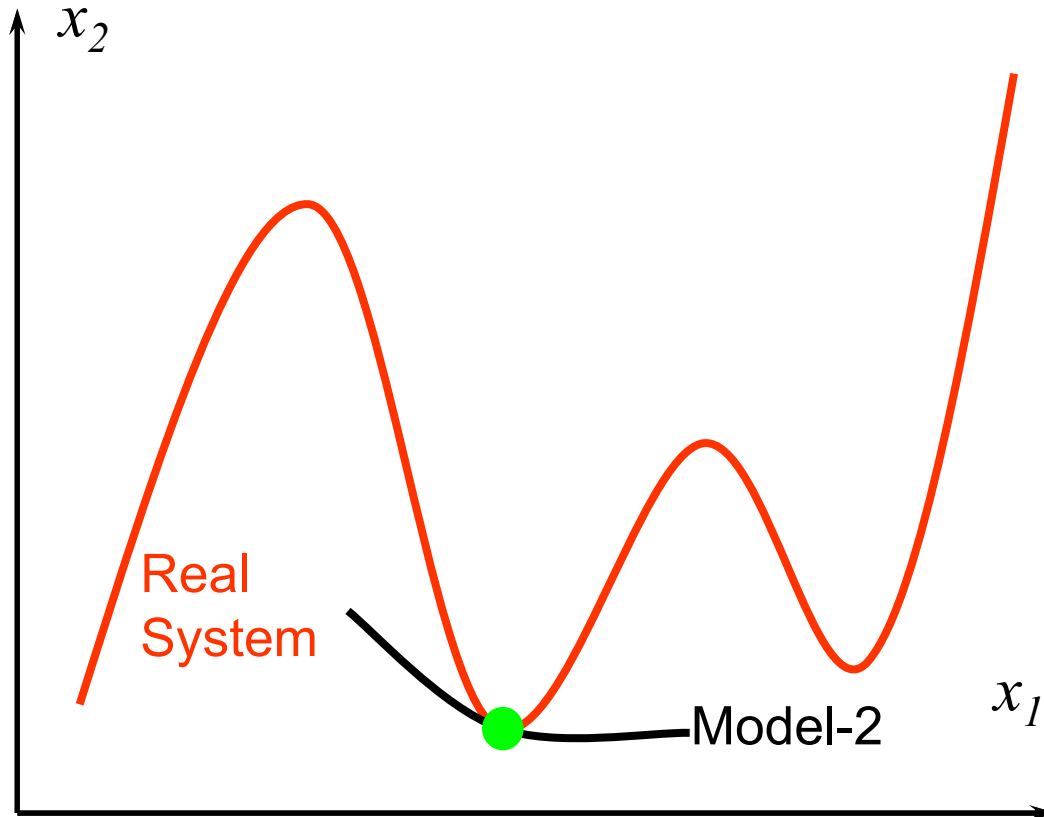
# Model Fit D



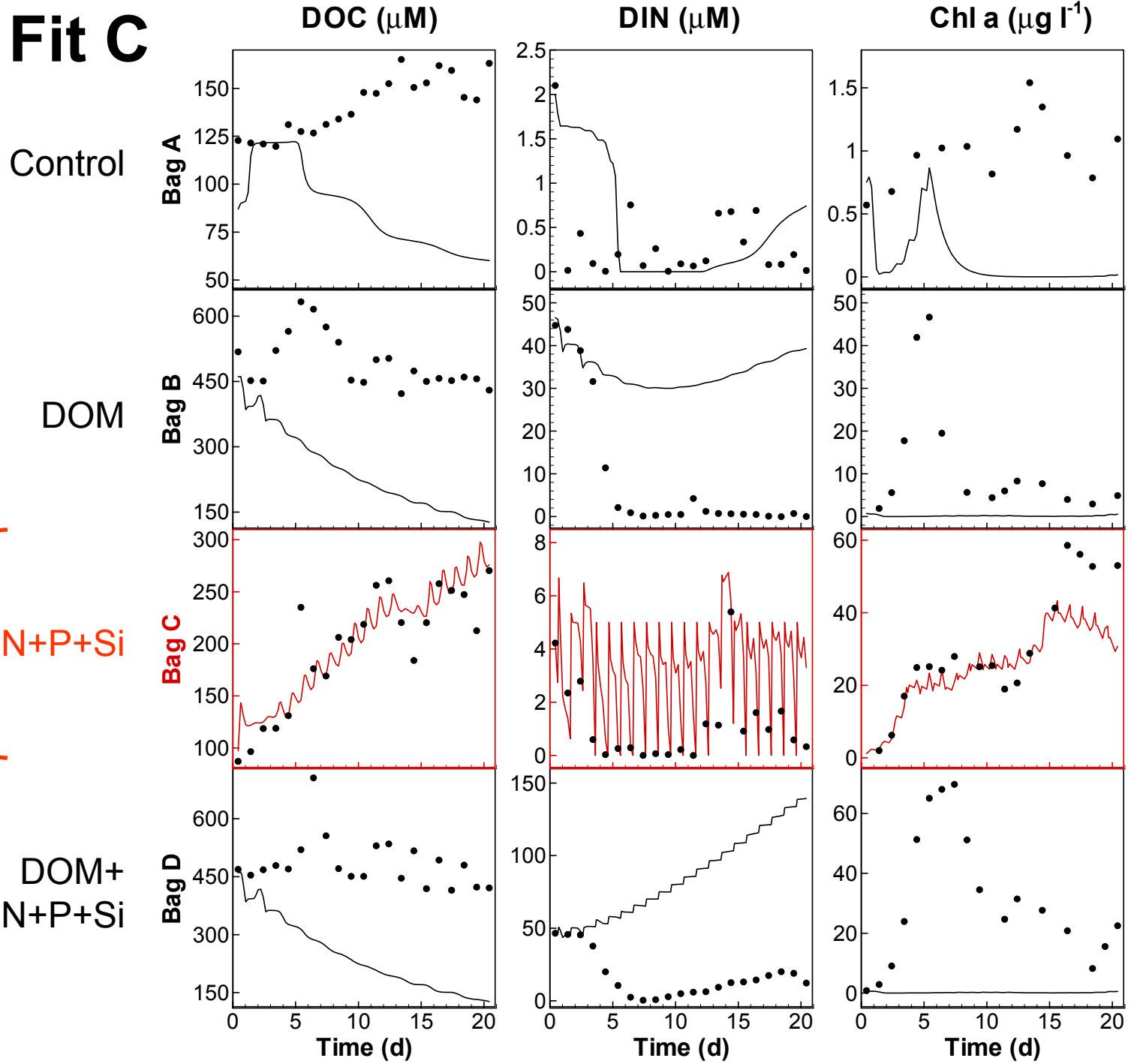
Fit Model To  
DOM+  
N+P+Si

# Recalibration

Models can be recalibrated about new a operating point, but again model is only locally valid

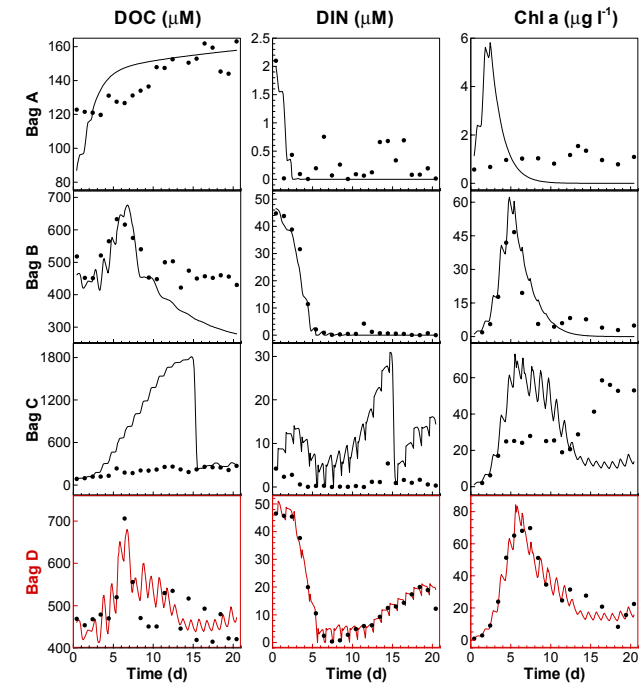
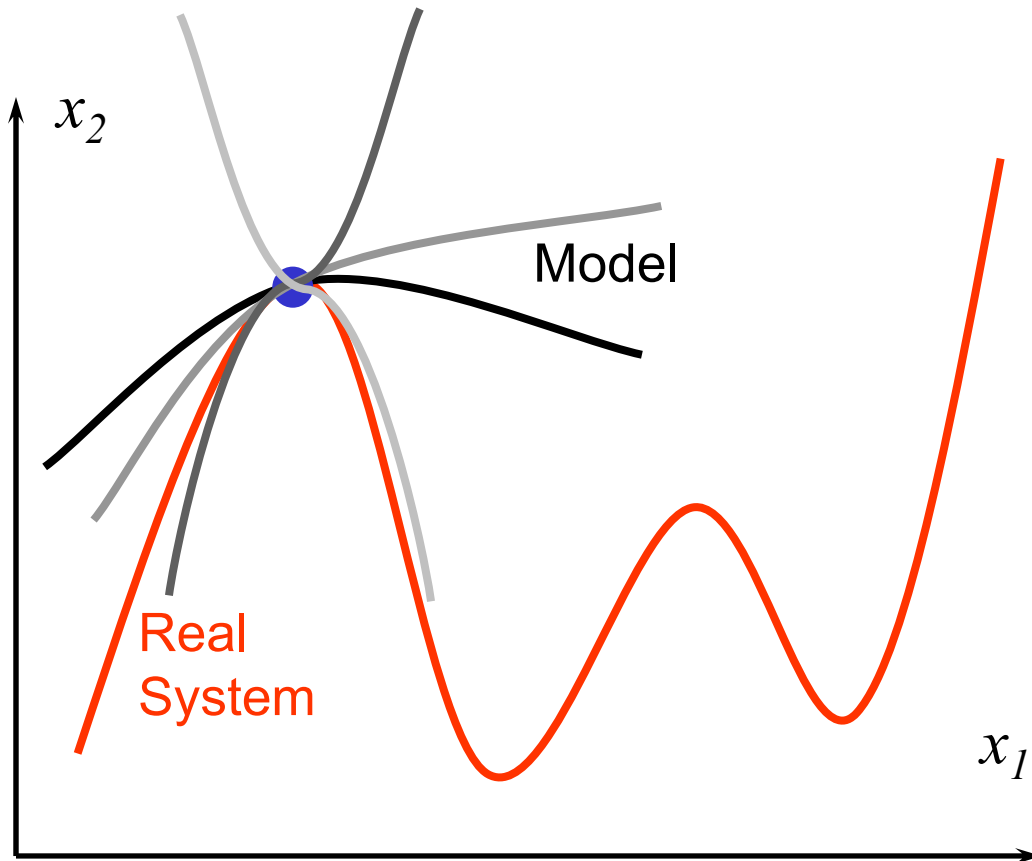


# Model Fit C



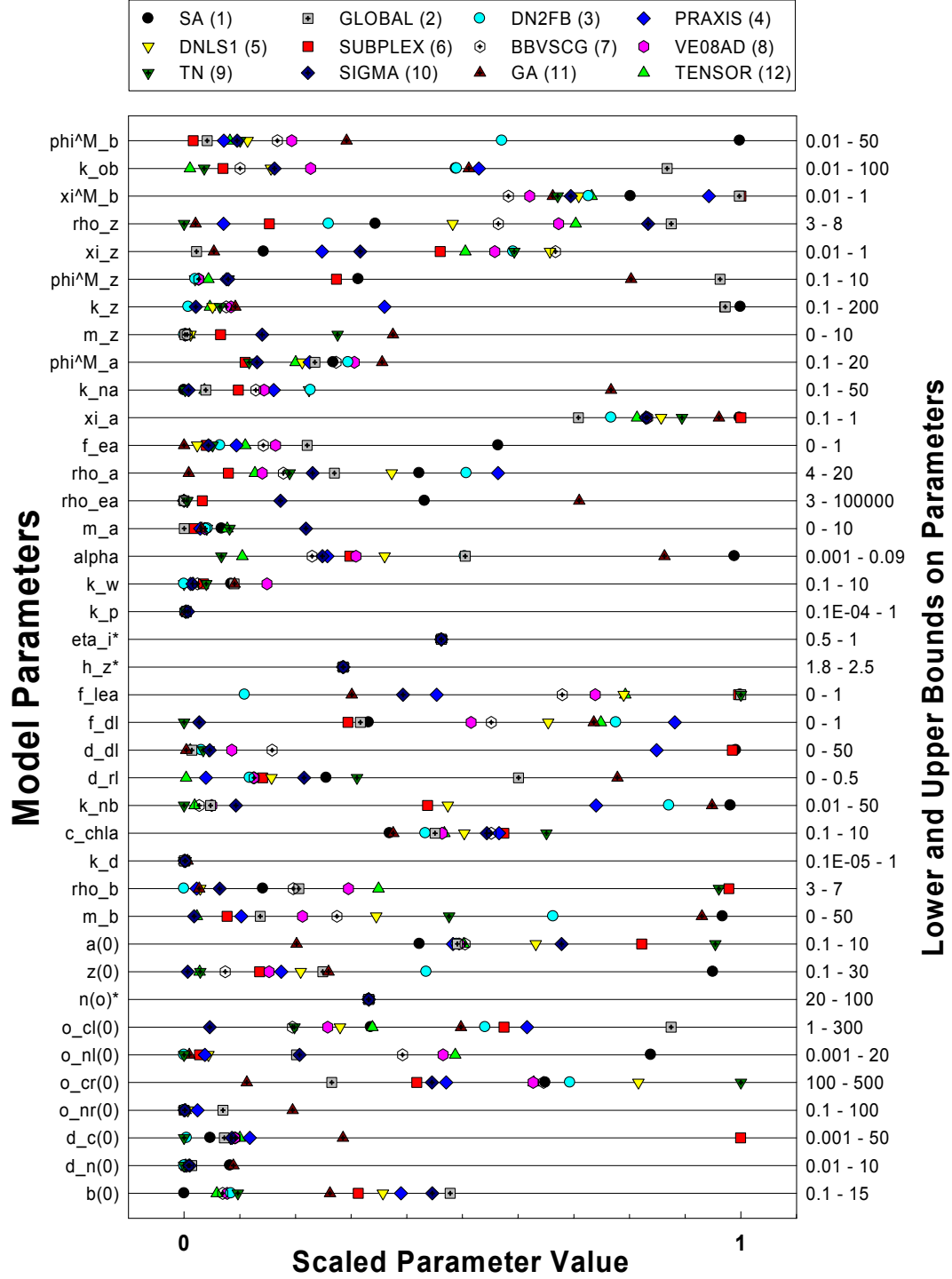
# No Unique Parameter Set

Many model parameterizations give similar fits, but dynamics differ radically outside calibration envelope.

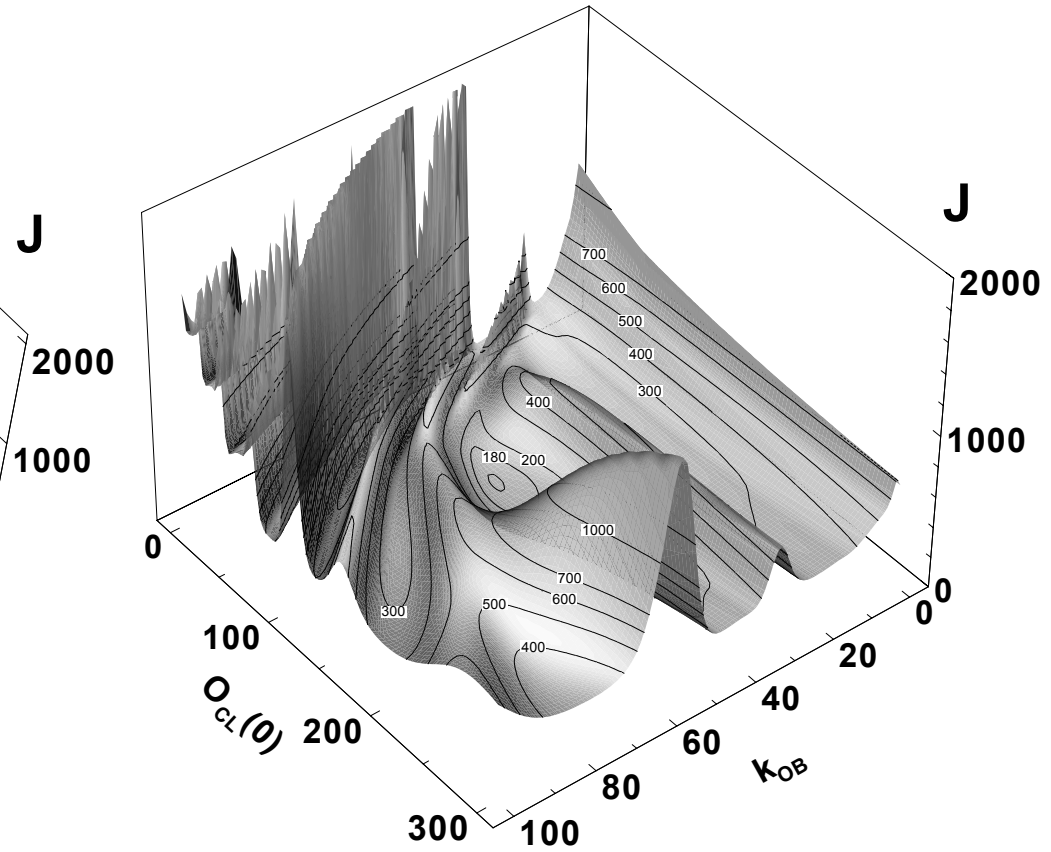
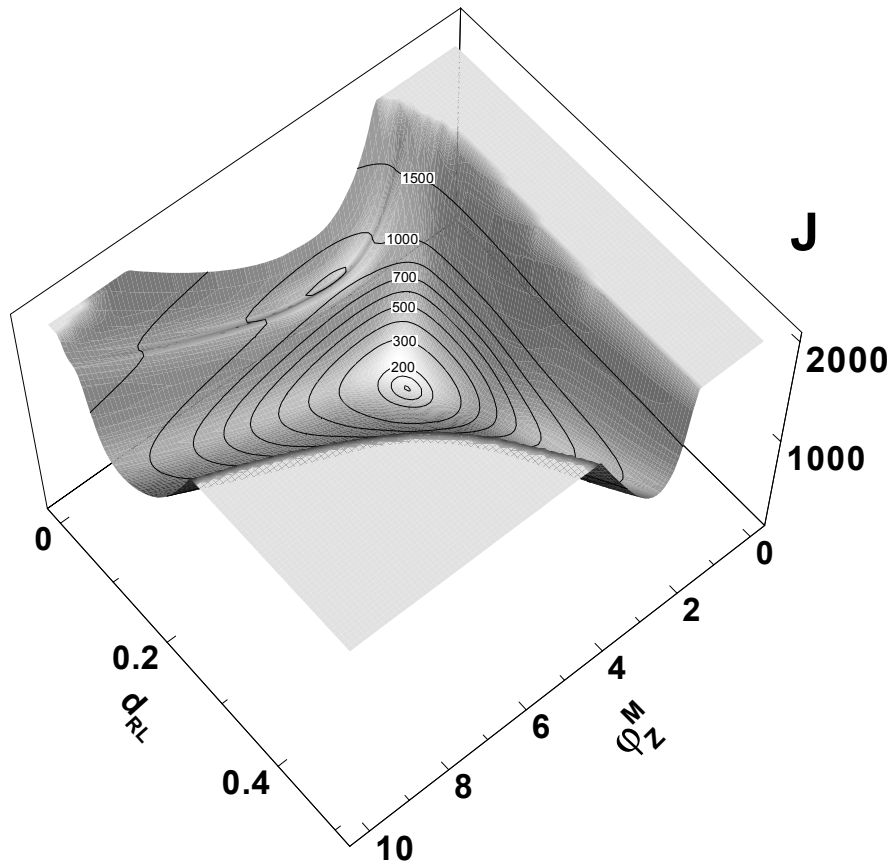


# Parameter Variability

Different model fits result in vastly different parameter values.



# Examples of Local Optima



Local optima have similar cost values,  $J$ , but are distributed throughout parameter space.

# Possible Solutions to Static Structure?

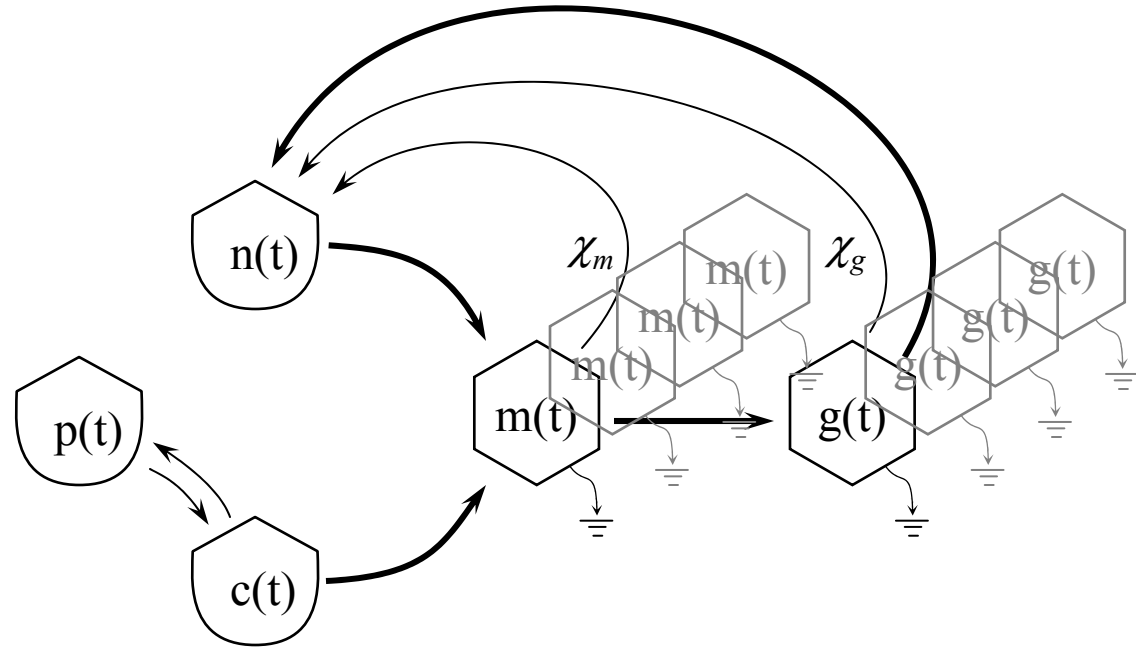
**Models need to capture shifts in community structure that occurs with changes in environmental conditions.**

## **Two possibilities:**

- *Stochastic modeling*
  - Initialize model with 10's to 1000's of “morphs” that are randomly parameterized.
  - Allow “natural selection” to cull population.
- *Optimization-based approaches*
  - Allow parameters to be variables.
  - Determine parameter values based on solution of optimization problem.



# Stochastic Model: Methanotroph Example



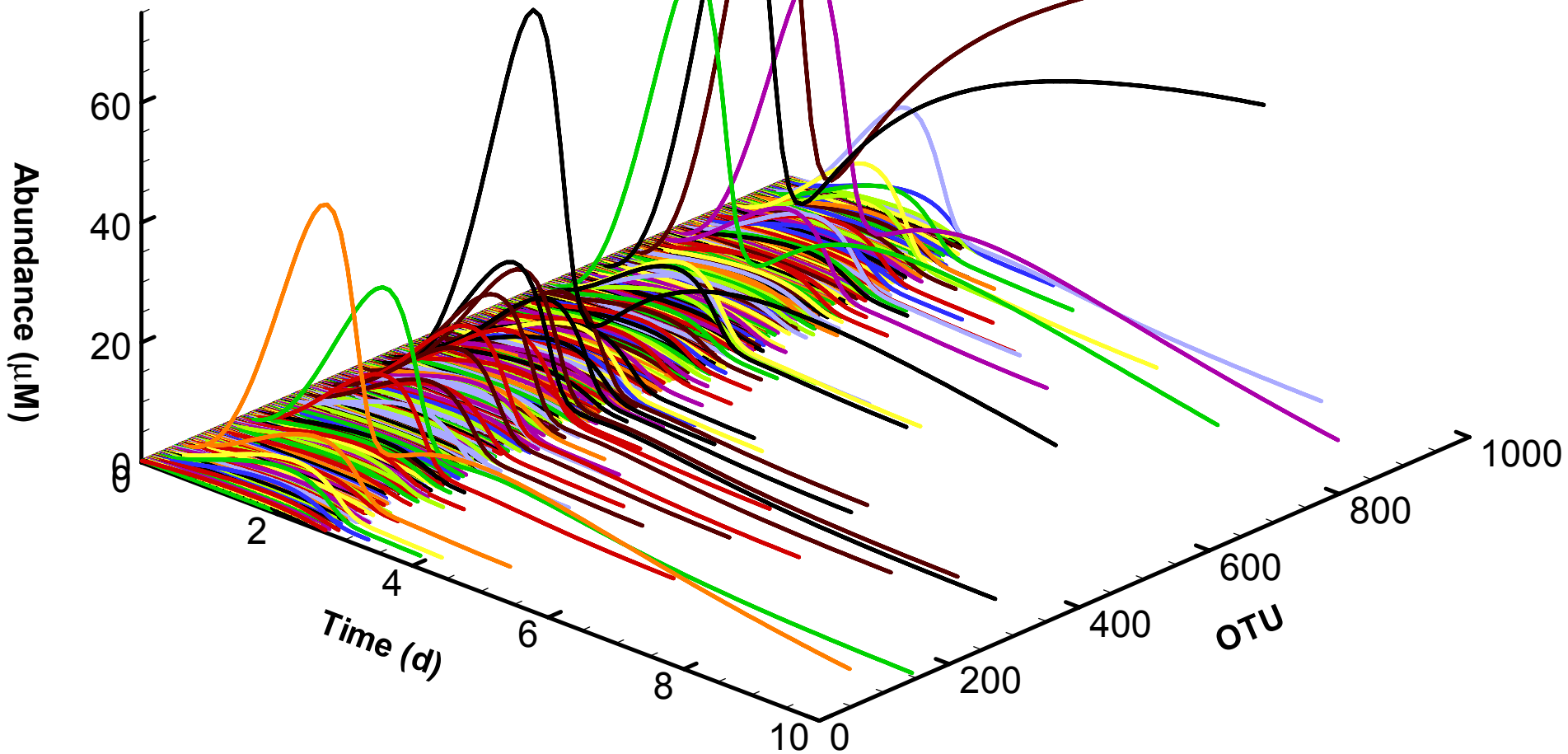
- n(t): Nitrogen
- p(t): Methane partial pressure
- c(t): Dissolved methane
- m(t): Methanotrophs
- g(t): Grazers

$$\varphi_m(n, c) = \frac{\boxed{\varphi_{m,\max}} n c}{(n + \boxed{k_{m,n}})(c + \boxed{k_{m,c}})}$$

$$\varphi_g(m) = \frac{\boxed{\varphi_{g,\max}} m^2}{(m + \boxed{k_{g,m}})^2}$$

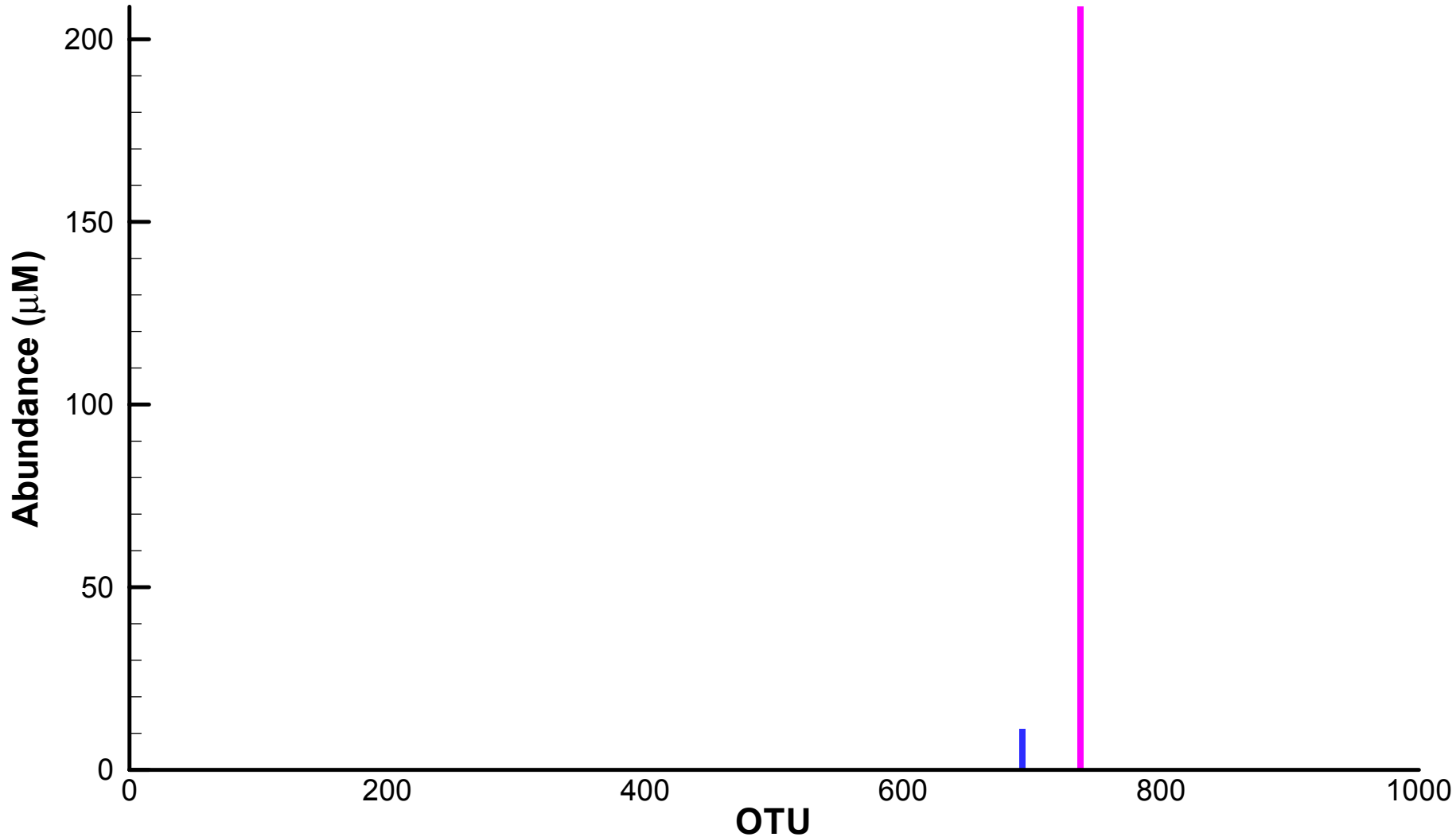
# OTU Dynamics (Methanotroph Morphs)

1000 Methanotrophs  
100 Grazers



# OTU Time Slices (Competitive Exclusion)

t = 99 d

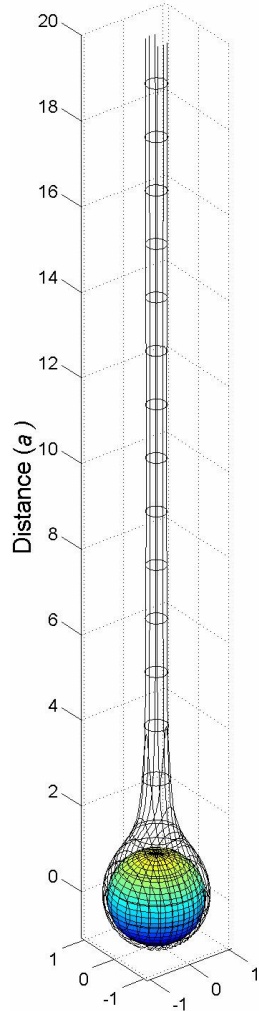


But this is a modeling artifact. No system is homogeneous!

# Spatiotemporal Heterogeneity

## DOM plumes

(Kiørboe and Jackson, 2001)

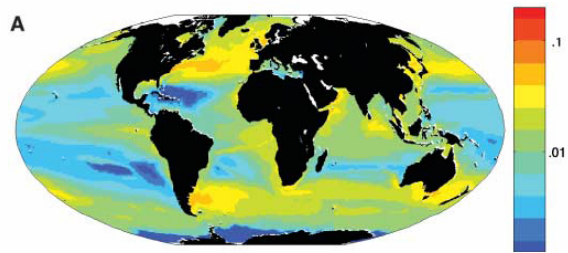


Need to use eddy resolving models, which are computationally intensive.

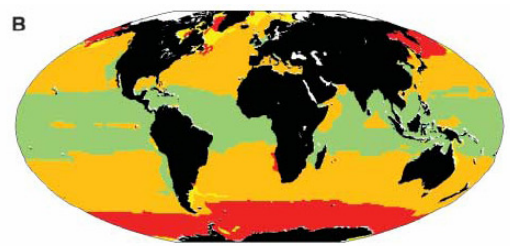
# “PZN” Example (Follows et al. 2007)

78 Phytoplankton Species  
Selection occurs via local conditions

Phytoplankton Biomass

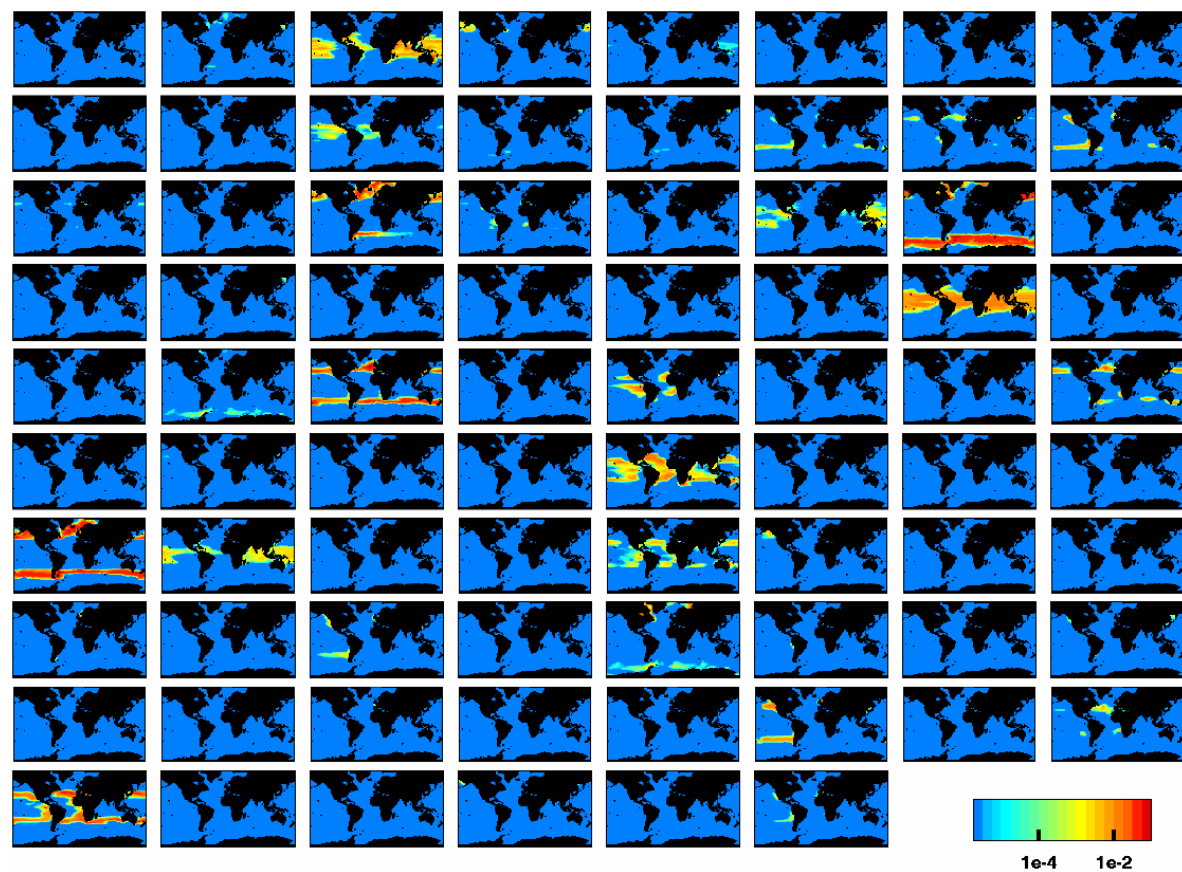


Four Phytoplankton Classes



- Prochlorococcus
- Small photoautotrophs
- Diatoms
- Large phytoplankton

78 Phytoplankton Morphs



# Parameter Relationships

Growth models use a form such as:

$$\frac{dP}{dt} = \varepsilon \mu^{Max} \left( \frac{N_1}{N_1 + K_{N_1}} \right) \cdots \left( \frac{N_n}{N_n + K_{N_n}} \right) + \cdots$$

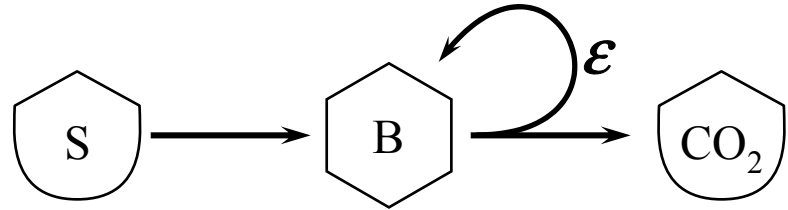
If random parameters are chosen independently, then the system will be dominated by morphs such as:

$$\varepsilon \rightarrow 1; \quad \mu^{Max} \rightarrow \infty; \quad K_{N_i} \rightarrow 0$$

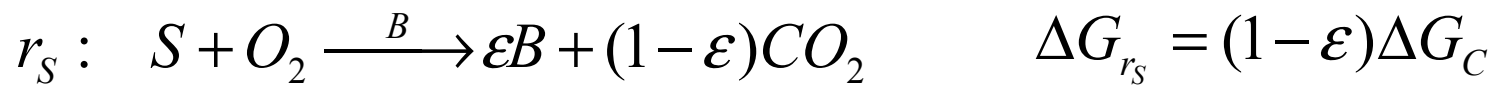
We know organisms can not achieve this, but what are the relationships?

Can optimization-based approaches work here?

# Efficiency vs. Growth Rate



$$\Delta G_f(S) \approx \Delta G_f(B)$$



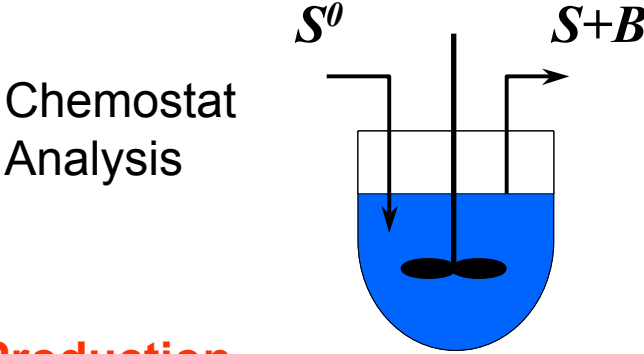
$$r_S = v^M B \underbrace{\left( \frac{S}{S + K_S} \right)}_{\text{Kinetic Force}} \underbrace{\left[ 1 - \exp\left( \frac{(1 - \epsilon) \Delta G_C}{RT\chi} \right) \right]}_{\text{Thermodynamic Force}} \quad (\text{cf. Jin, Q. and Bethke, C.M. 2003})$$

$$r_G = \epsilon r_S \quad \text{Rate of biomass synthesis (Growth)}$$



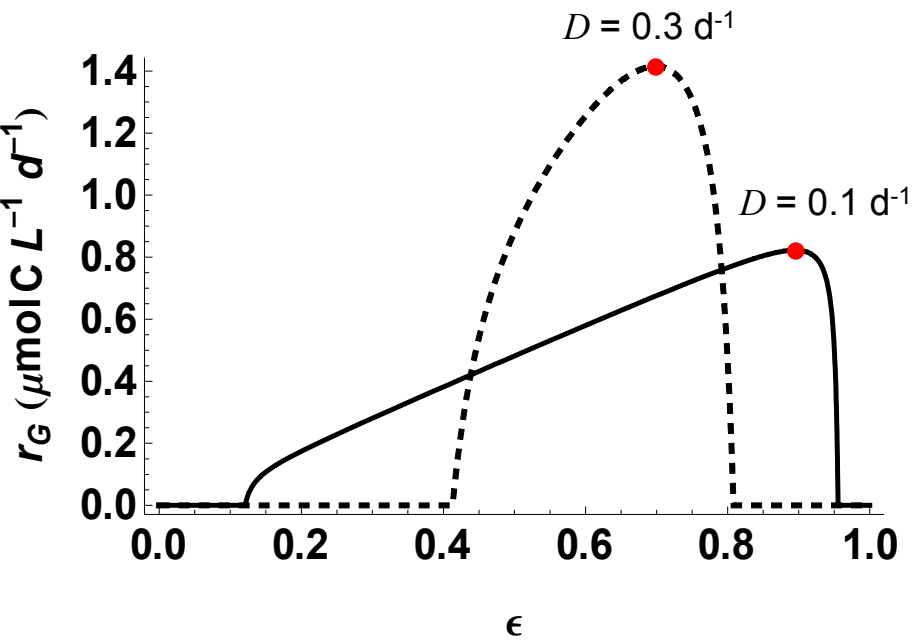
# Maximize Growth vs. Entropy Production

Select growth efficiency,  $\epsilon$ , base on either maximizing growth rate (MGR) or entropy production (MEP). See Dewar (2003) for later.



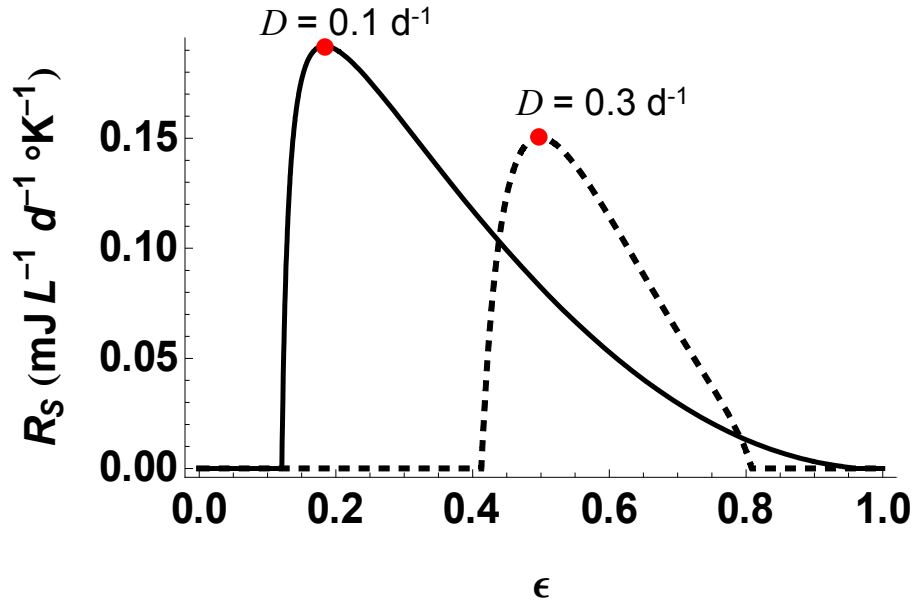
## Max Biomass Production

$$\max \epsilon r_S$$



## Max Entropy Production

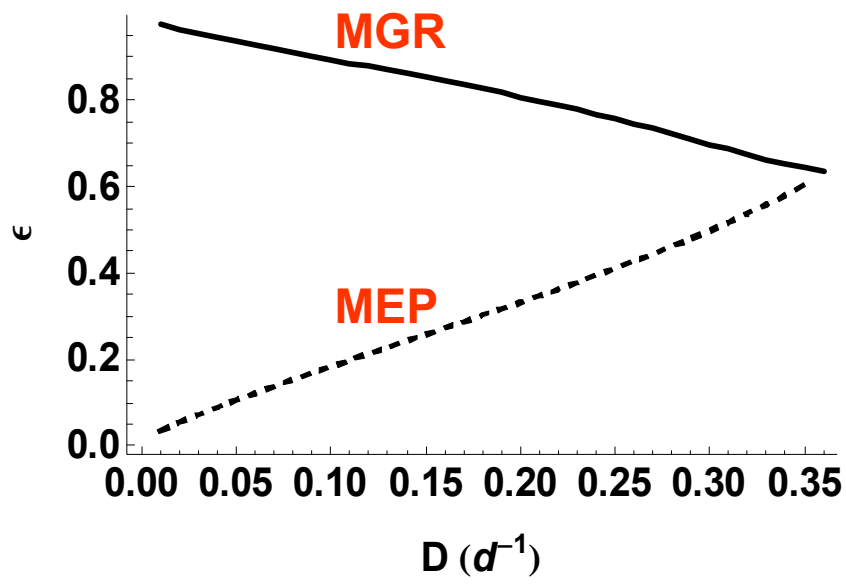
$$\max (1 - \epsilon) \Delta G_C r_S$$



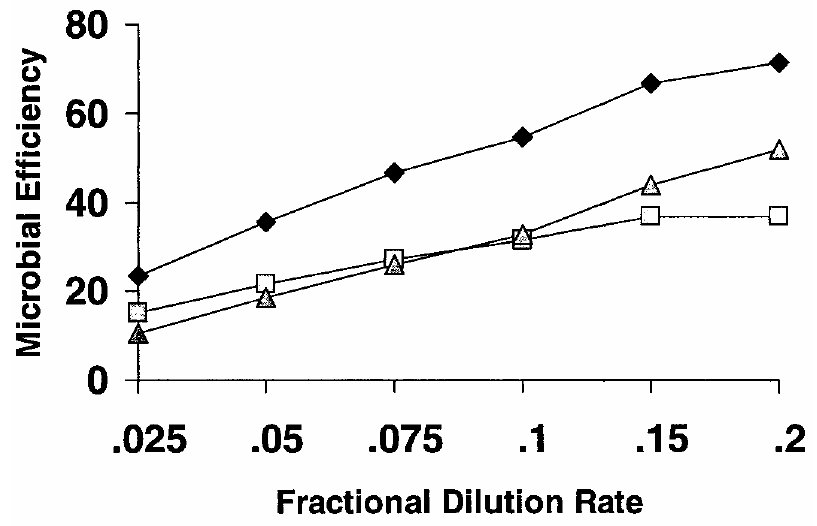
# Growth Efficiency Trends: MGR vs. MEP

**MGR:** Efficiency is high and goes down with increasing  $D$

**MEP:** Efficiency is low and goes up with increasing  $D$



Effect of dilution rate on microbial growth efficiency of ruminant microbial community (Meng et al. 1999).



# Summary

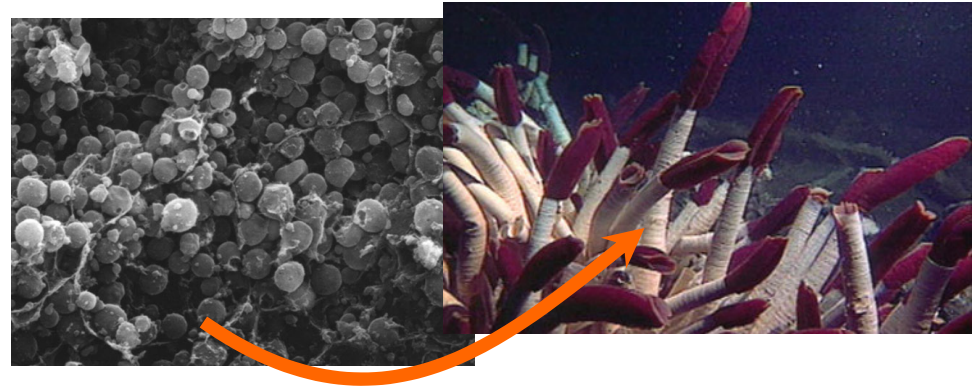
- Communities change composition as environmental drives change.
- Standard models require recalibration at each new operating point.
- Consequently, structurally fixed models can not capture full dynamics.
- Possible solutions:
  - Use stochastic models to capture true ecosystem diversity.
  - Use optimization approaches to determine model “constants”.
- However, how do you solve without using 100's or 1000's of compartments or imbedding a nonlinear optimization problem, both of which are computationally intensive?

# Function Transcending Organism Boundaries

Mycorrhizae

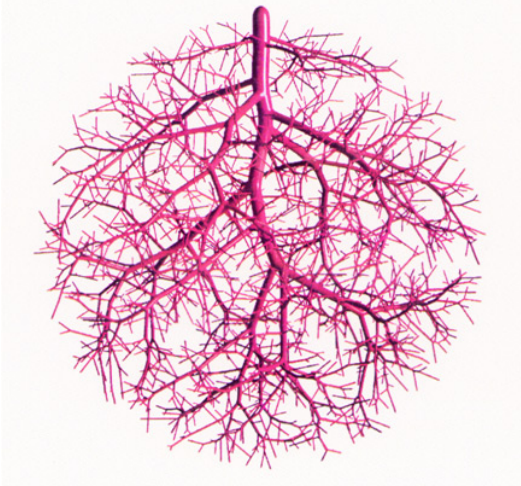


Sulfur bacteria in *Riftia*

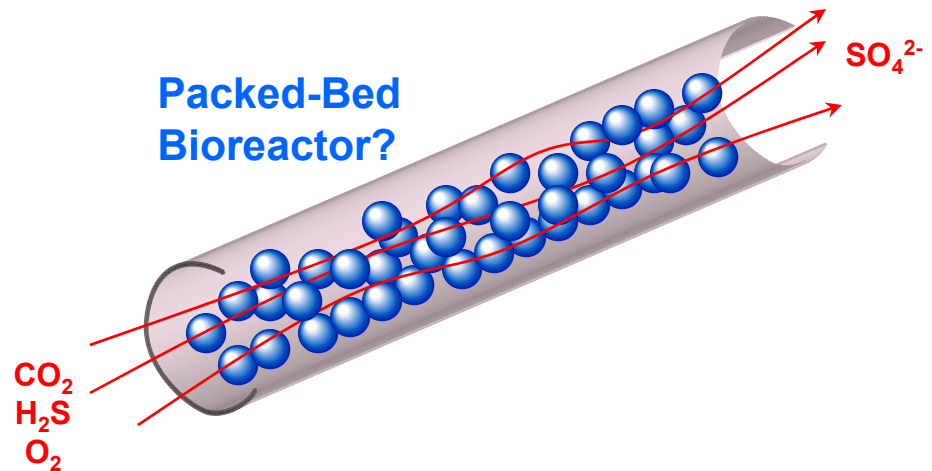


From an MEP perspective, these systems look like this:

Space-Filling Fractal Network



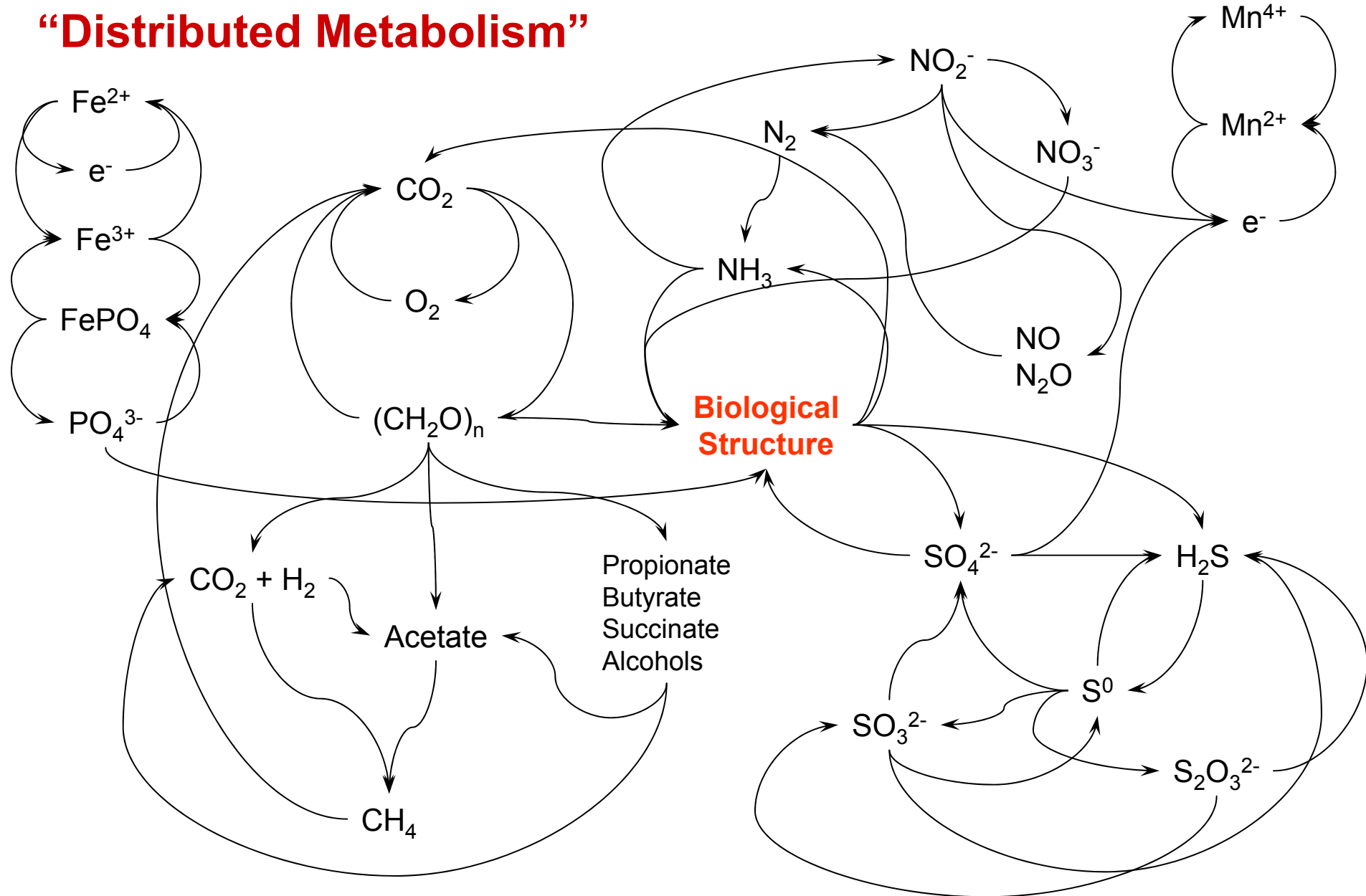
Packed-Bed Bioreactor?



Perhaps modeling with a functional emphasis would be better

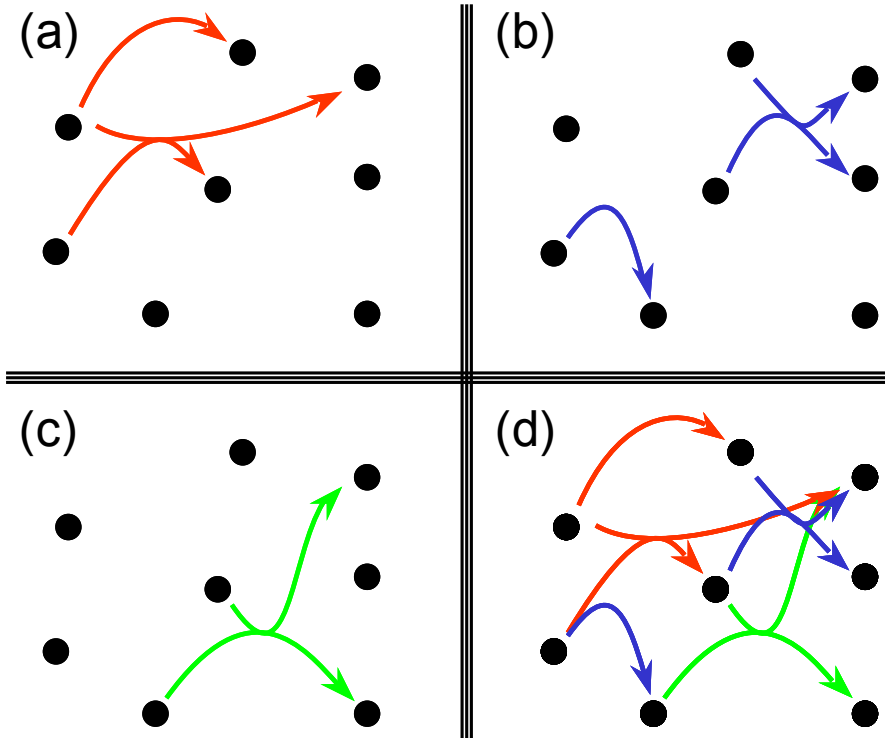
# Ecosystem Metabolic Network

## “Distributed Metabolism”

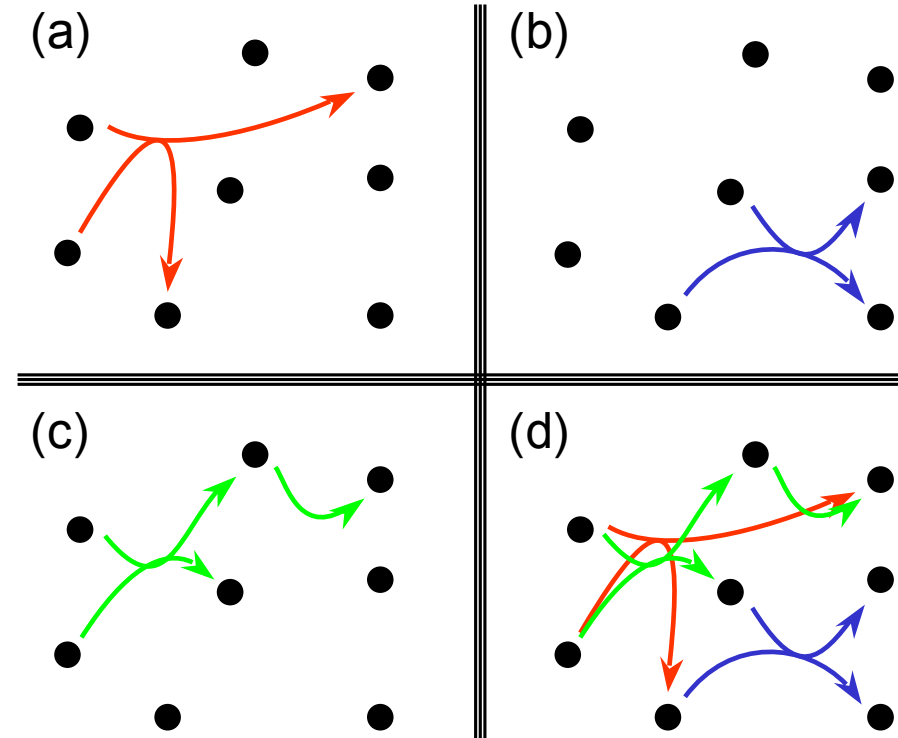


# Many Food Web Configurations

## Complementary Network 1

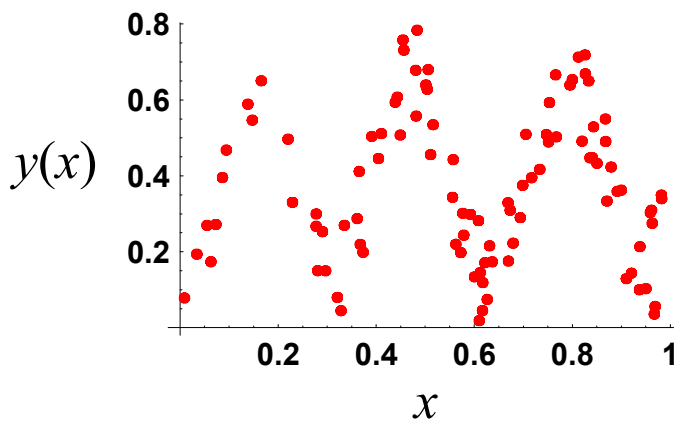


## Complementary Network 2



# Local and Global Optima Example

Raw Data

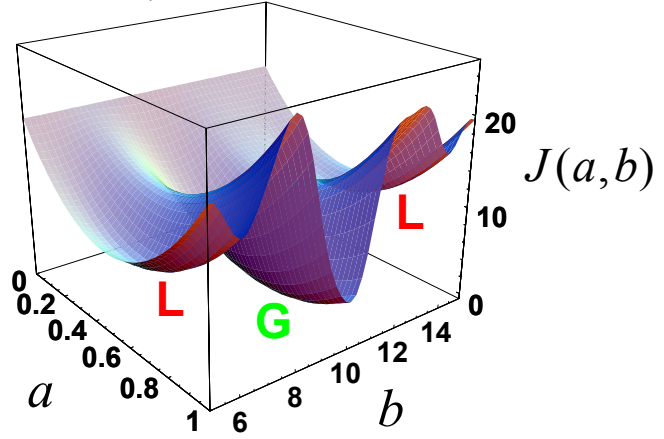


Model

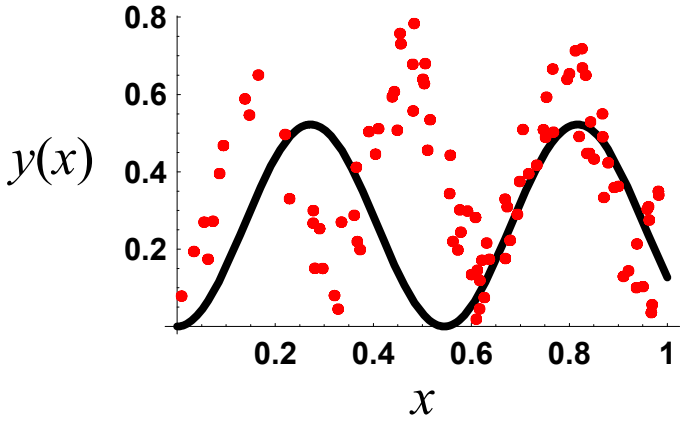
$$\hat{y}(x) = a \sin^2(bx)$$



$$J(a,b) = \sum_i (y(x_i) - \hat{y}(x_i))^2$$



Local Optima Solution



Global Optima Solution

