Improving Marine Ecosystem Models: Use of Data Assimilation and Mesocosm Experiments

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ASLO Meeting

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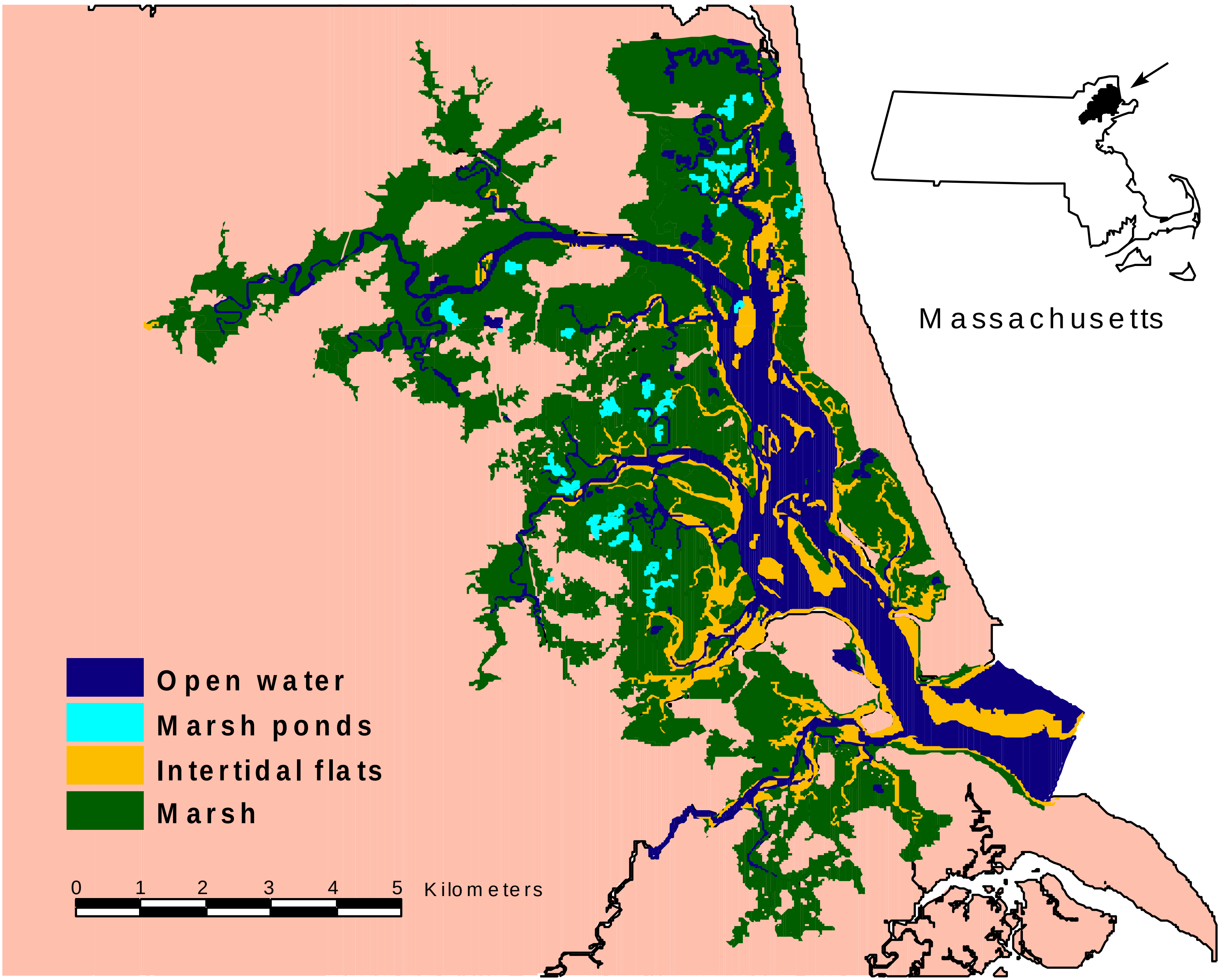
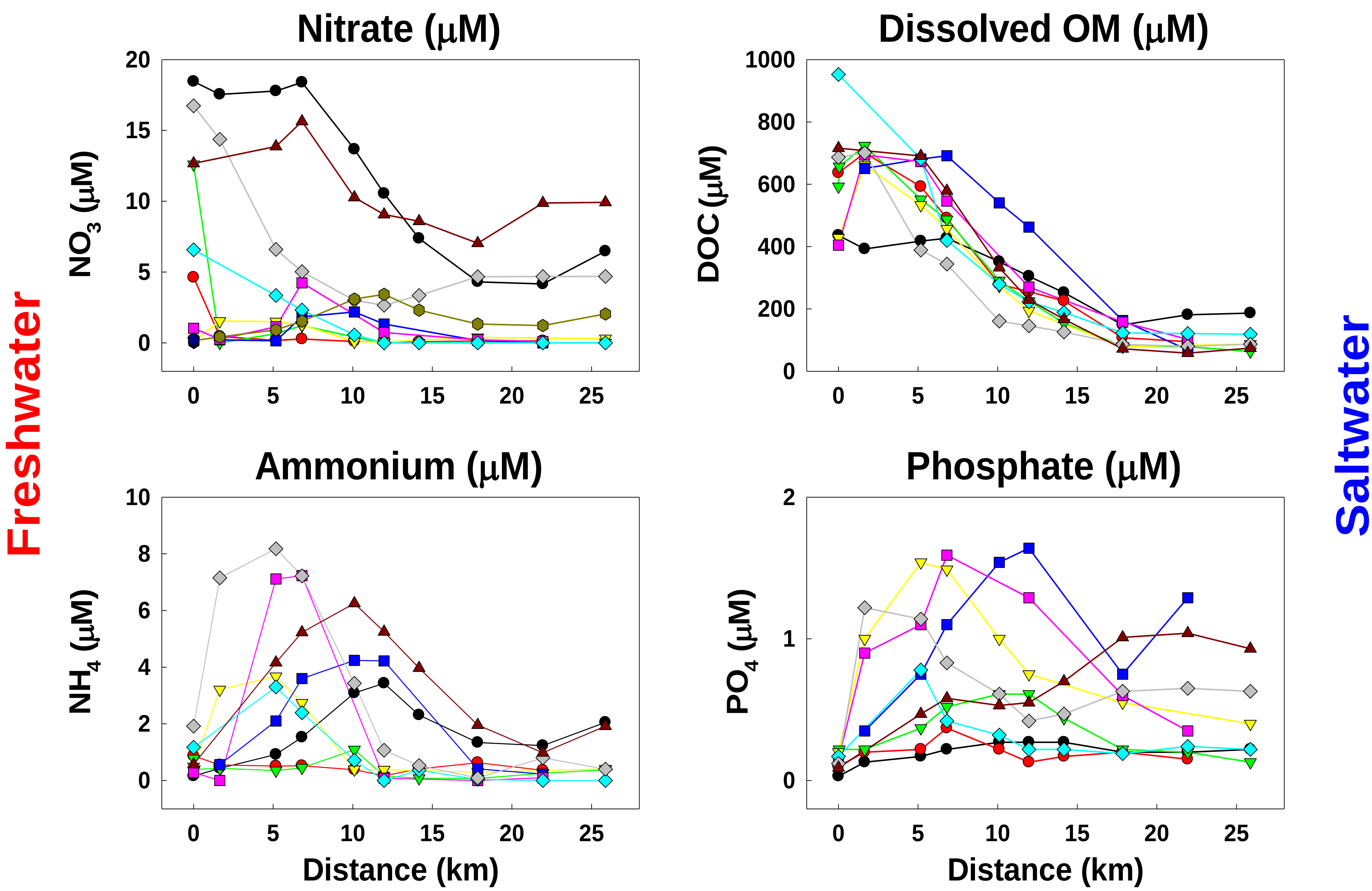
Ecosystems Center

Marine Biological Laboratory, Woods Hole MA

Plum Island Estuary (PIE) LTER Site



Nutrient Transects Along Parker River And Plum Island Sound, 1994



Mesocosm Experiment

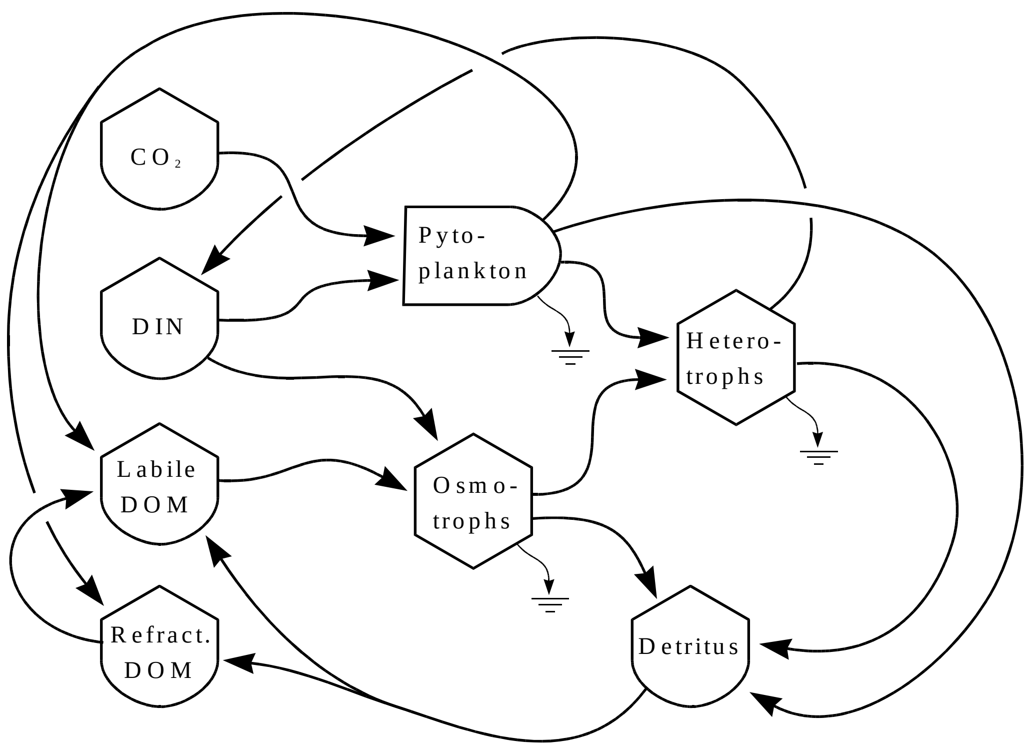
- **Additions:**
  - NO_3 (5 μM), PO_4 (0.5 μM), Si (7 μM)
  - Leaf litter leachate (300 μM DOC)

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

- **Samples Taken:**
  - NO_3, NH_4, PO_4, Si, O_2 DIC
  - PAR
  - POC, PON, DOC, DON
  - Chl a
  - PP (^{14}C and O_2 incubations)
  - Bacterial No. and productivity
  - Phyto- and zooplankton counts
  - $DI^{13}C$, $DO^{13}C$, $DO^{15}N$
  - Size fractionated $\delta^{13}C$ and $\delta^{15}N$

Mesocosm Food Web Model

- Aggregated, coupled C and N model
- Emphasis on OM processing
- Holling type II and III growth kinetics



- State Eqns: 10
  - Auto. C, N
  - Osomo. C, N
  - Hetero. C, N
  - Detritus C
  - Detritus N
  - DIN N
  - DOM-L C
  - DOM-L N
  - DOM-R C
  - DOM-R N
- Parameters
  - 29 Kinetic
  - 10 Initial cond.

Data Assimilation Problem

- **State Model:** $\mathbf{x}(t;\mathbf{k})$

$$\frac{d\mathbf{x}(t;\mathbf{k})}{dt} = \mathbf{f}(\mathbf{x}(t;\mathbf{k}), t;\mathbf{p}), \quad \mathbf{x}(t_0;\mathbf{k}) = \mathbf{x}_0$$

- **Mapping to Observations:** $\mathbf{y}(t)$

$$\mathbf{y}(t) = \mathbf{h}(\mathbf{x}(t,\mathbf{k}), t;\mathbf{p}) + \boldsymbol{\nu}(t)$$

e.g., $P_{OC}(t) = A(t) + H(t) + B(t) + D_C(t)$

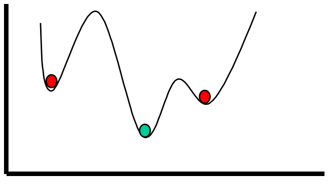
- **Objective Function:** $J(\mathbf{k})$

$$\min_{\mathbf{k}} \; J(\mathbf{k}) = \int_{t_0}^{t_f} \left(\mathbf{h}(\mathbf{x}(t;\mathbf{k}), t;\mathbf{p}) - \mathbf{y}(t)\right)^{\mathrm{T}} \boldsymbol{\Psi}(t)^{-1} \left(\mathbf{h}(\mathbf{x}(t;\mathbf{k}), t;\mathbf{p}) - \mathbf{y}(t)\right) dt$$

$\boldsymbol{\Psi}(t)$: **Measurement error**

Optimization Problem

- "Curse of Dimension"
  - Classic algorithms assume J quadratic in neighborhood of minimum
- Gradient Required for Classic Algorithms
  - Need $\frac{\partial J(\mathbf{k})}{\partial \mathbf{k}}$, but J implicit in $\mathbf{k}$
  - Use Adjoint equations
- Global and Local Minima



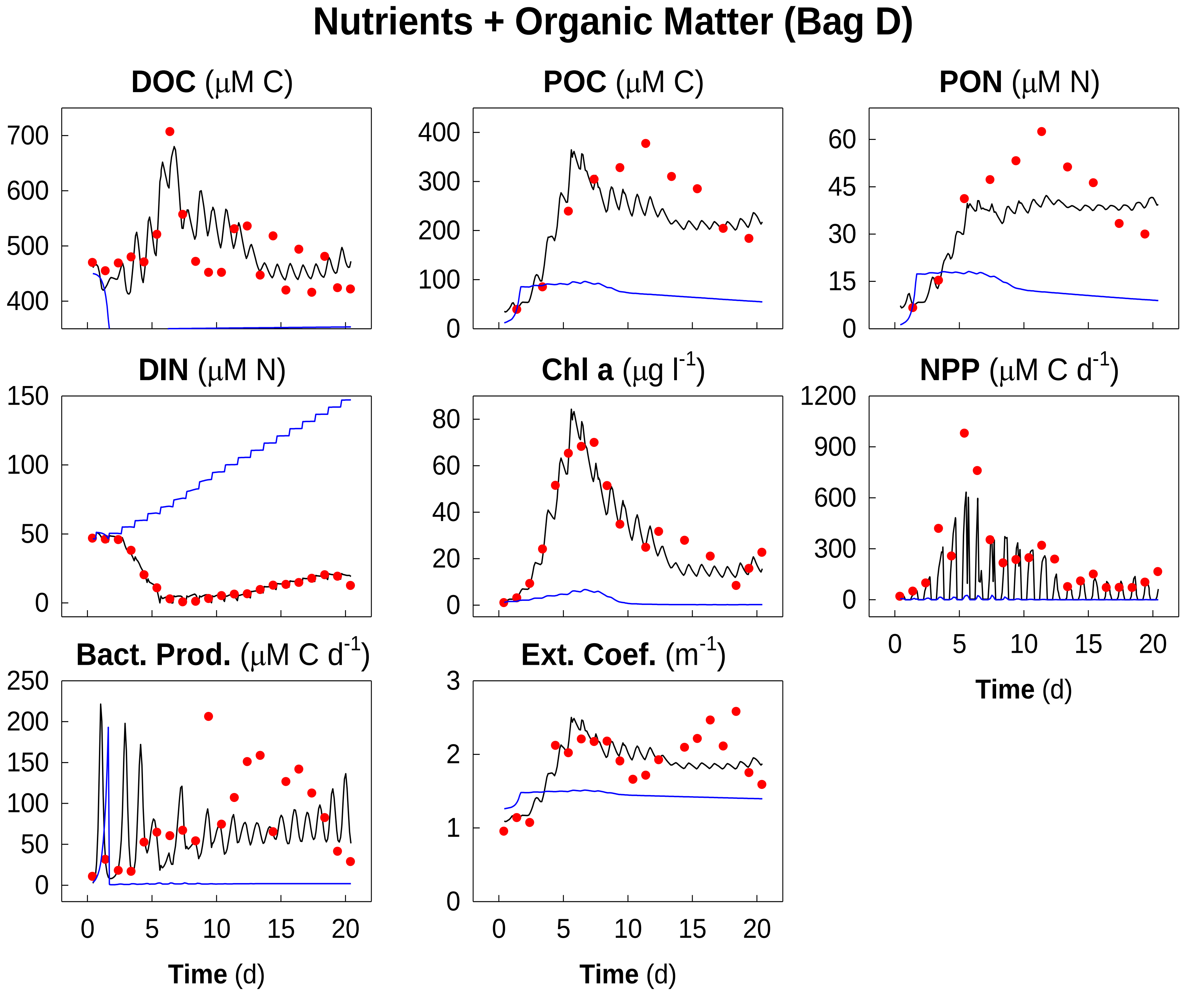
  - Area of active research
  - Test both local and global routines
- Parameter Observability and Dependency
  - Perturbation analysis
  - SVD at minimum (only locally valid!)
- Parameter Scaling and Bounds
  - Use Sin^2 transform

Optimization Routines Tested

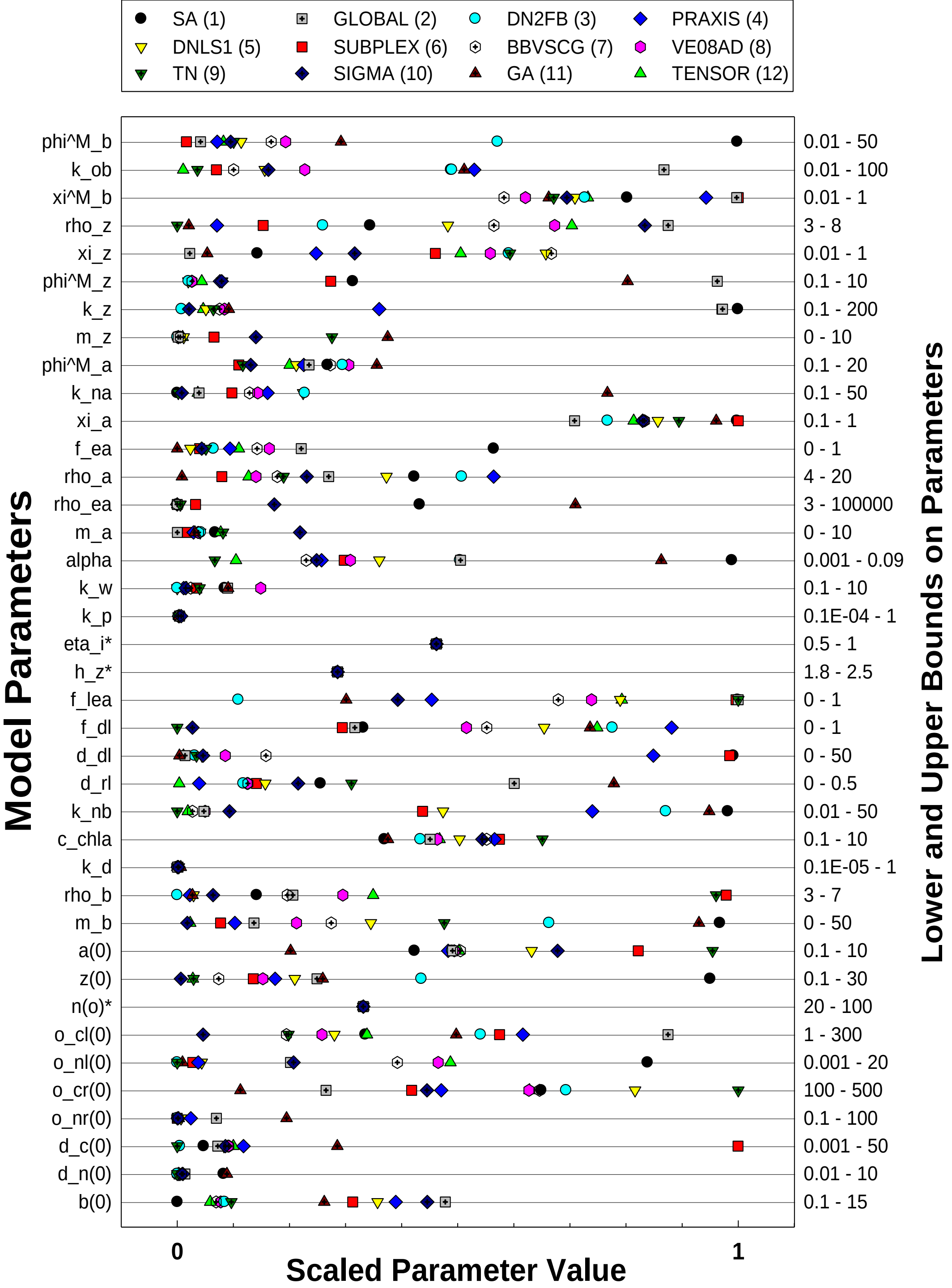
Routine	Algorithm	Optima	Gradient
<u>CG Routines</u>			
PRAXIS	Powel's Conjugate gradient	Local	No
DN2FB	Adaptive Newton	Local	Yes
DNLS1	Levenberg-Marquardt	Local	Yes
BBVSCG	quasi-Newton and CG	Local	Yes
VE08	Quasi-Newton	Local	Yes
TN	Truncated Newton	Local	Yes
TENSOR	Tensor method	Local	Yes
<u>Non CG Routines</u>			
SUBPLEX	Modified simplex	Local	No
SA	Simulated annealing	Global	No
SIGMA	Stochastic differential equations	Global	No
GLOBAL	QN with stochastic searching.	Global	No
GA	Genetic algorithm	Global	No

Optimization Results

Routine	Function Calls	CPU Time (hr)	Final Cost $J(t_f)$
SA	350000	253	170
GLOBAL	181273	347	204
DN2FB	3537	7.77	237
PRAXIS	8455	6.65	248
DNLS1	566	1.15	258
SUBPLEX	6946	5.1	292
BBVSCG	169	0.74	337
VE08	241	1.35	345
TN	539	2.13	471
SIGMA	179422	485	546
GA	200020	321	577
TENSOR	57902	278	693

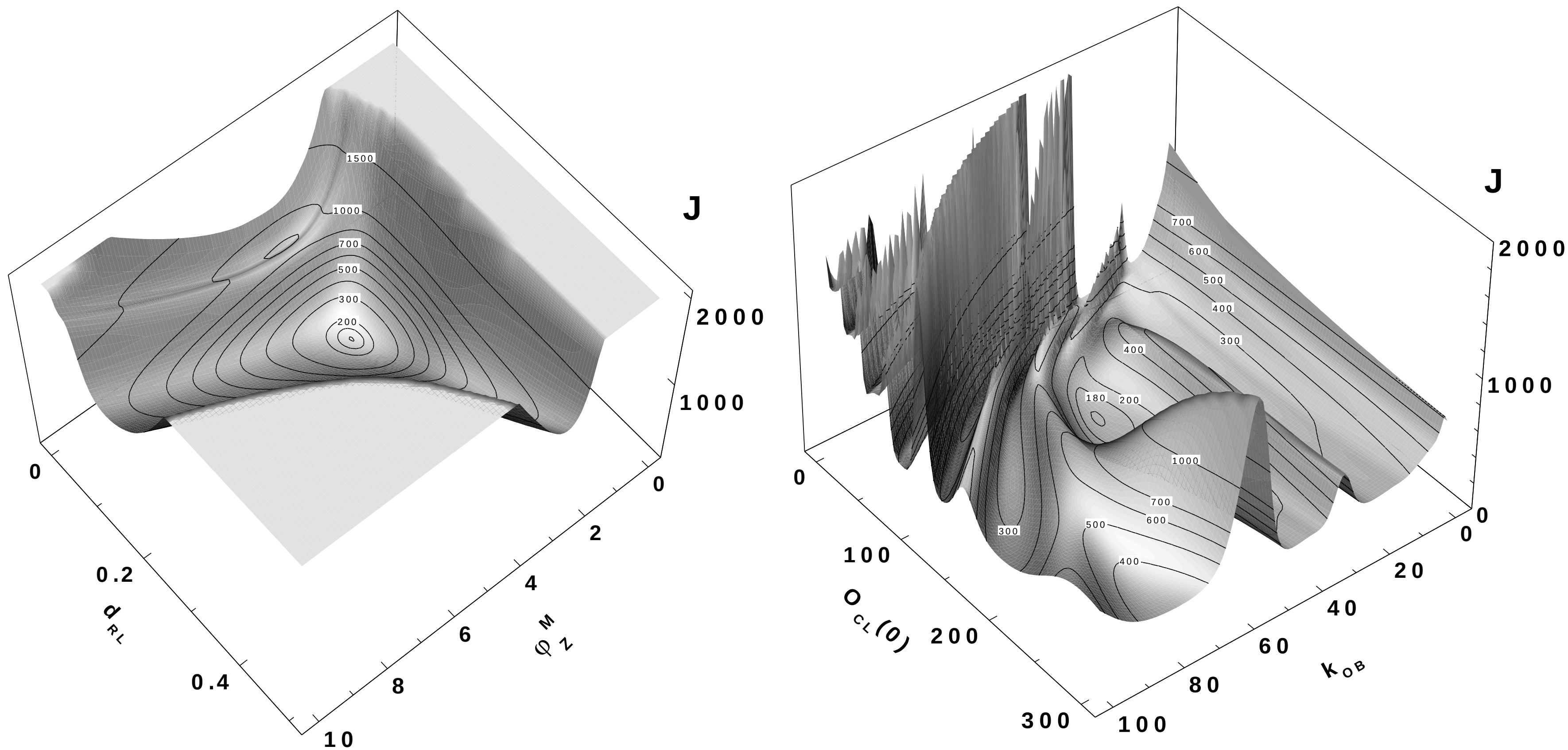


Nutrients + Organic Matter (Bag D)
DOC (μM C)
POC (μM C)
PON (μM N)
DIN (μM N)
Chl a (μg l-1)
NPP (μM C d-1)
Bact. Prod. (μM C d-1)
Ext. Coef. (m-1)
Time (d)



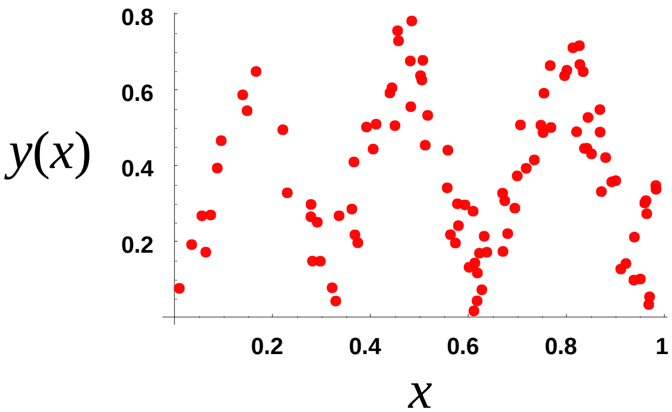
SA (1)
GLOBAL (2)
DN2FB (3)
PRAXIS (4)
DNLS1 (5)
SUBPLEX (6)
BBVSCG (7)
VE08AD (8)
TN (9)
SIGMA (10)
GA (11)
TENSOR (12)
Model Parameters
phi^M_b
k_ob
xi^M_b
rho_z
xi_z
phi^M_z
k_z
m_z
phi^M_a
k_na
xi_a
f_ea
rho_a
rho_ea
m_a
alpha
k_w
k_p
eta_i*
h_z*
f_lea
f_dl
d_dl
d_rl
k_nb
c_chla
k_d
rho_b
m_b
a(0)
z(0)
n(o)*
o_cl(0)
o_nl(0)
o_cr(0)
o_nr(0)
d_c(0)
d_n(0)
b(0)
Lower and Upper Bounds on Parameters
0.01 - 50
0.01 - 100
0.01 - 1
3 - 8
0.01 - 1
0.1 - 10
0.1 - 200
0 - 10
0.1 - 20
0.1 - 50
0.1 - 1
0 - 1
4 - 20
3 - 100000
0 - 10
0.001 - 0.09
0.1 - 10
0.1E-04 - 1
0.5 - 1
1.8 - 2.5
0 - 1
0 - 1
0 - 50
0 - 0.5
0.01 - 50
0.1 - 10
0.1E-05 - 1
3 - 7
0 - 50
0.1 - 10
0.1 - 30
20 - 100
1 - 300
0.001 - 20
100 - 500
0.1 - 100
0.001 - 50
0.01 - 10
0.1 - 15
0
1
Scaled Parameter Value

Examples of 2D Ojbective Function Surfaces



Local and Global Optima

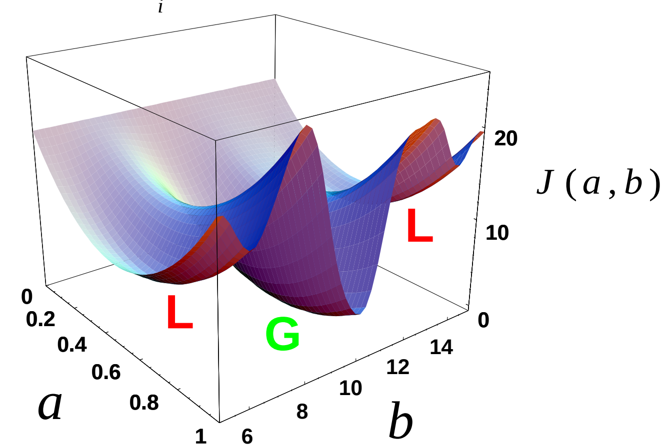
Raw Data



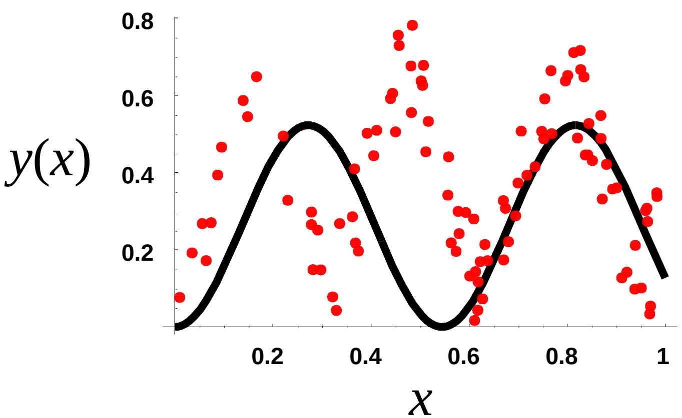
Model

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

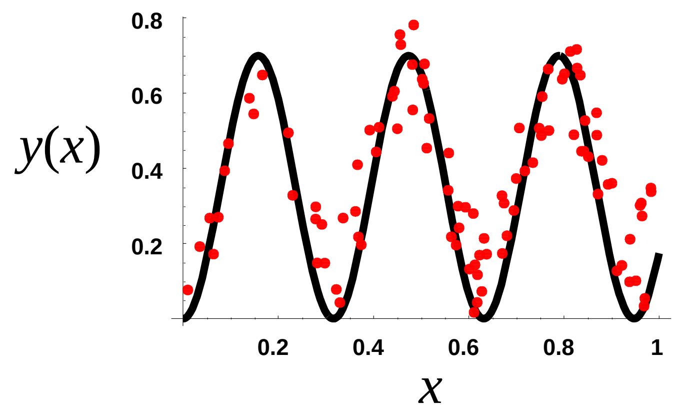
$$J(a,b) = \sum_i \left(y(x_i) - \hat{y}(x_i) \right)^2$$



Local Optima Solution

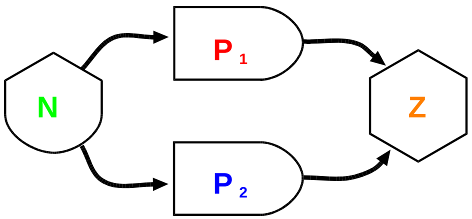


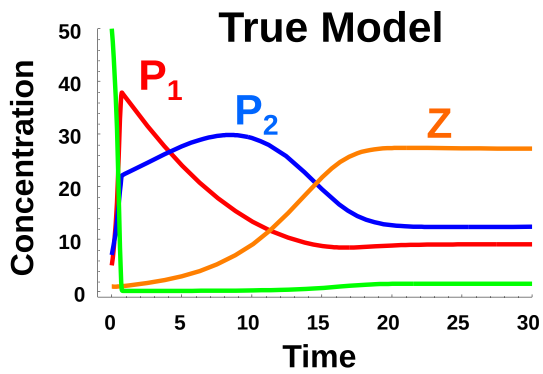
Global Optima Solution



Model Errors

- Aggregation Error

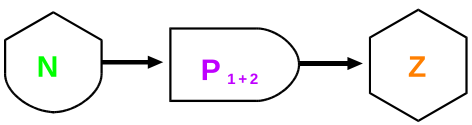


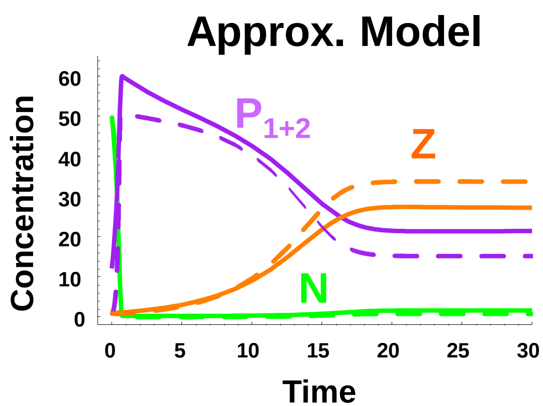


True parameter values

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

$P_{1+2} = P_1 + P_2$



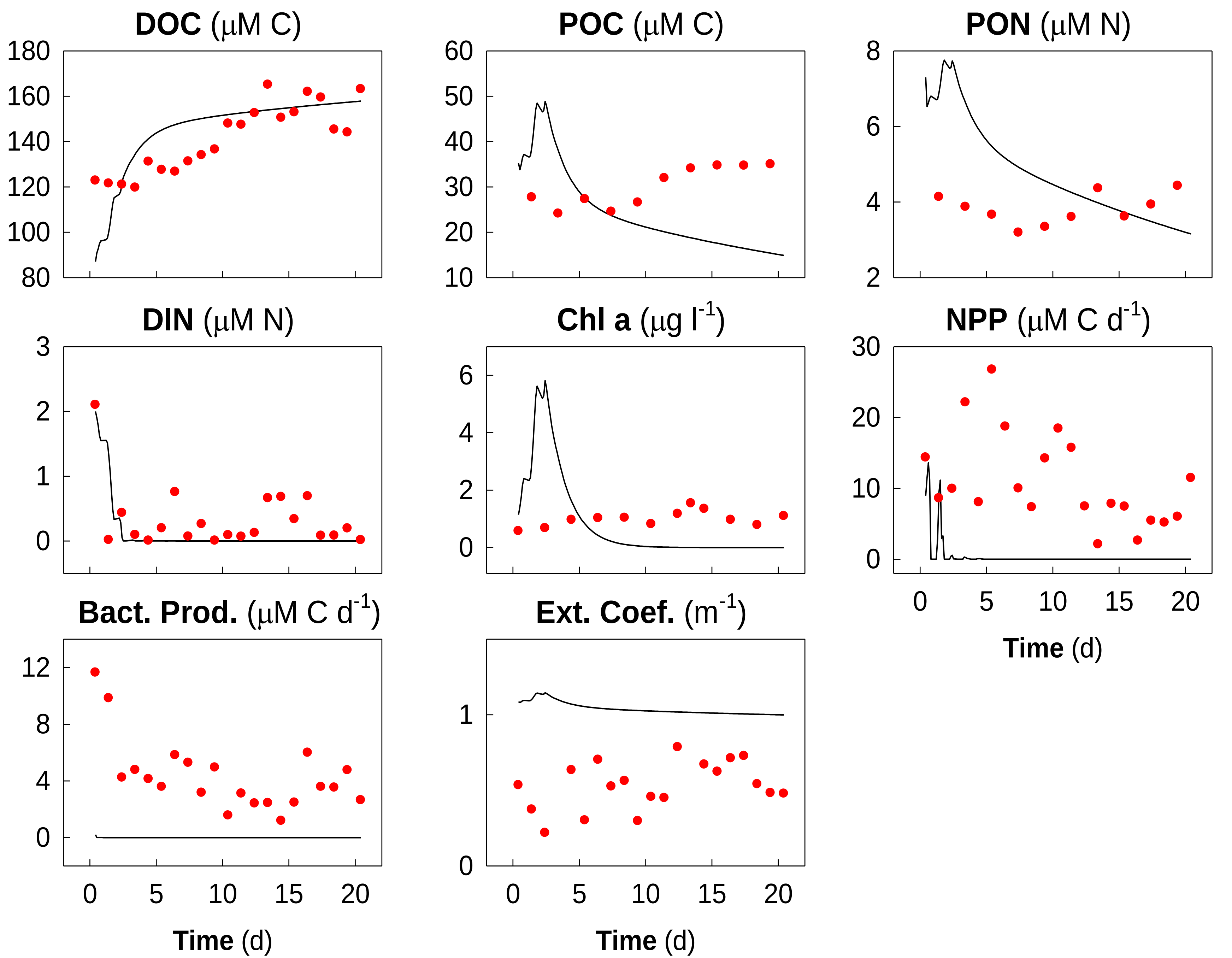


Estimated aggregated parameter values

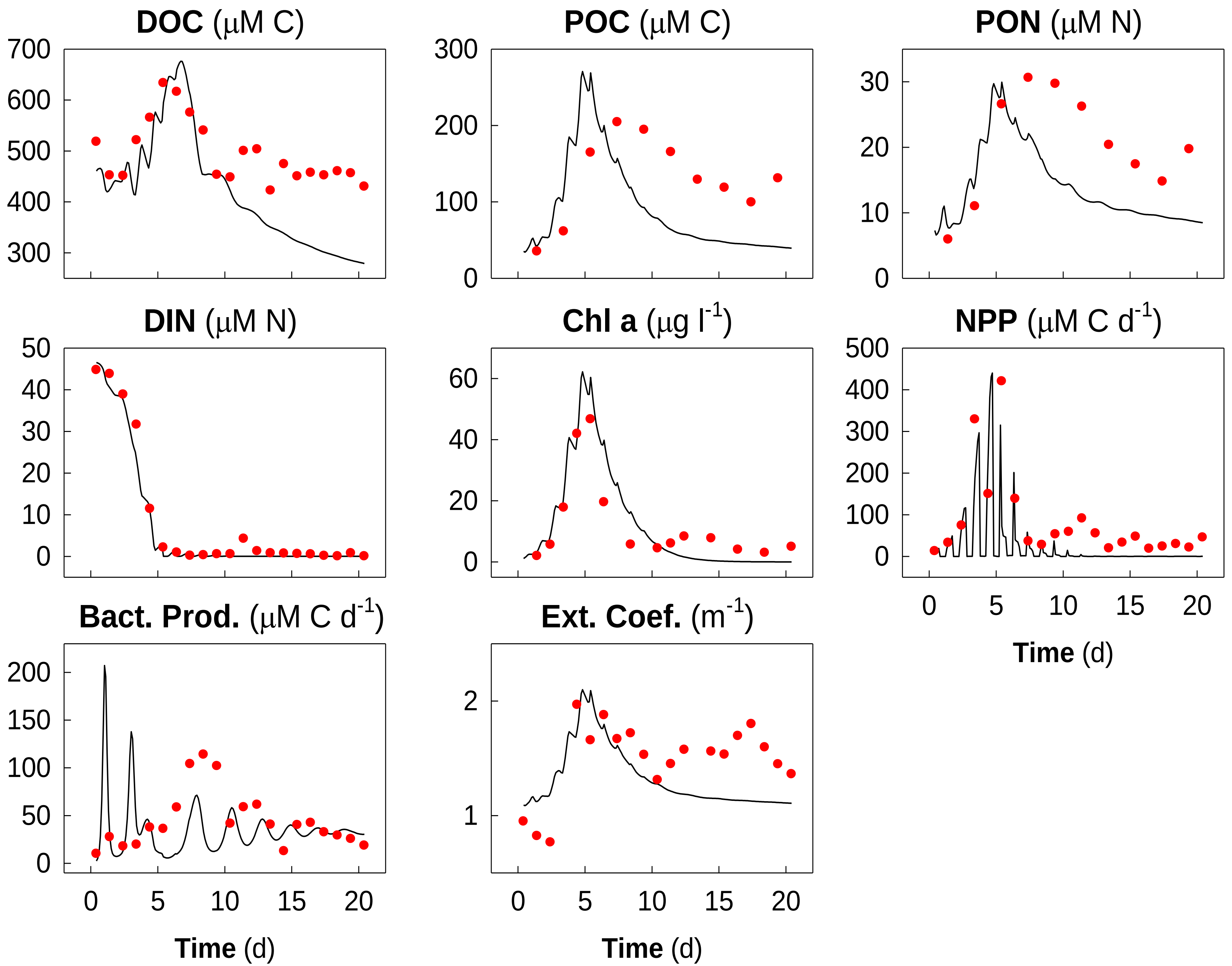
	V^M	K_s	$P(0)$
P_{1+2}	8.2	3.2	1

- Process Errors
  - Organic matter production and consumption.
  - Constant parameter values, such as C:N ratio of phytoplankton.
  - Mortality closure scheme.
  - Etc.

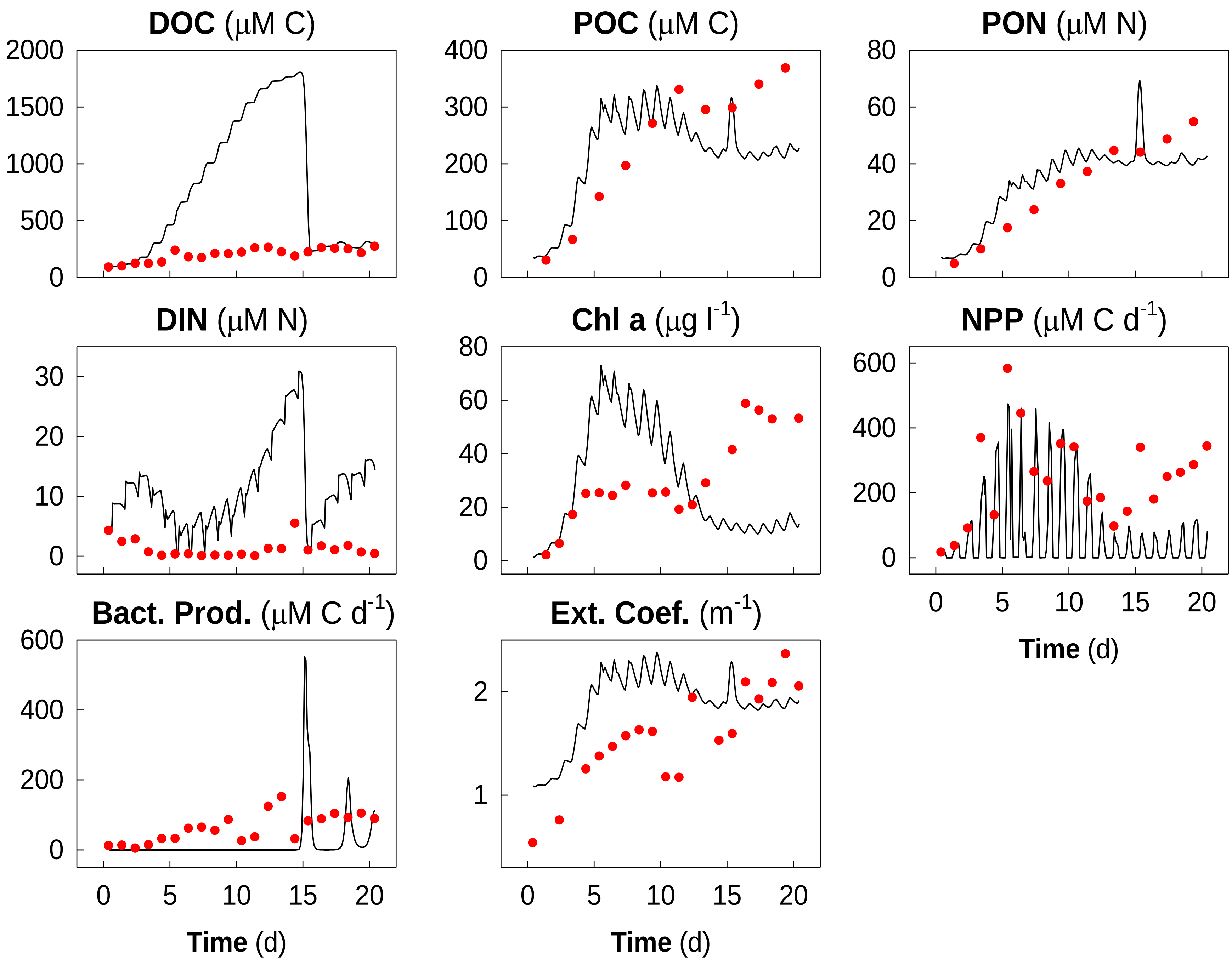
Control (Bag A with Bag D Parameters)



Organic Matter Only (Bag B with Bag D Parameters)



Inorganic Nutrients Only (Bag C with Bag D Parameters)



Conclusions

- Mesocosms useful for process based modeling
  - However, should separately model bag walls, etc.
- Optimization Routines
  - Simulated annealing, if computation limits permits
  - PRAXIS (no Grad.) or Levenberg-Marquardt (w/ Grad.) routines
  - Adjoint useful for computationally intense problems
- Integrate model development with experimental observations
- Improve model robustness based on aggregation techniques
  - Holistic versus reductionist approach
- Establish modeling benchmarks

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