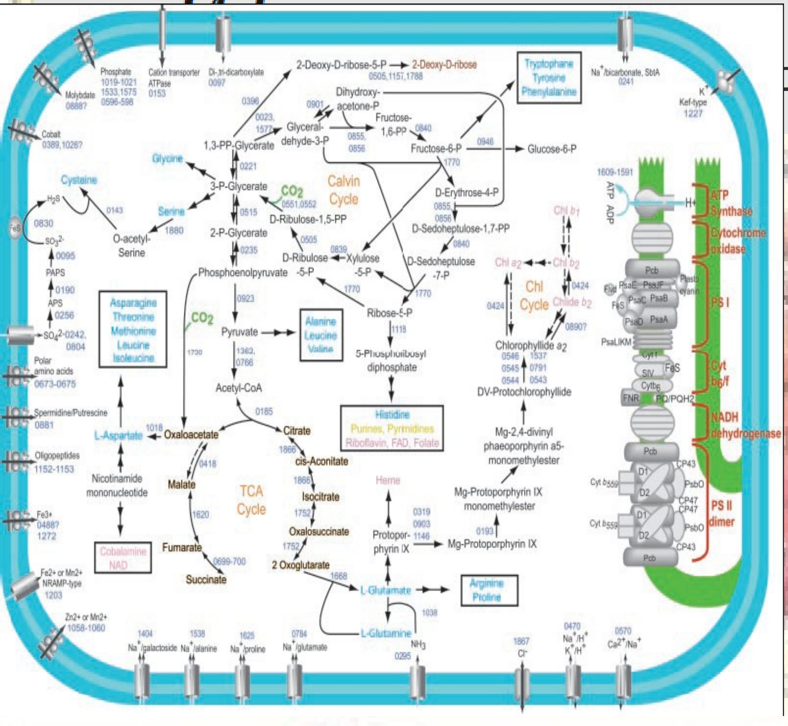
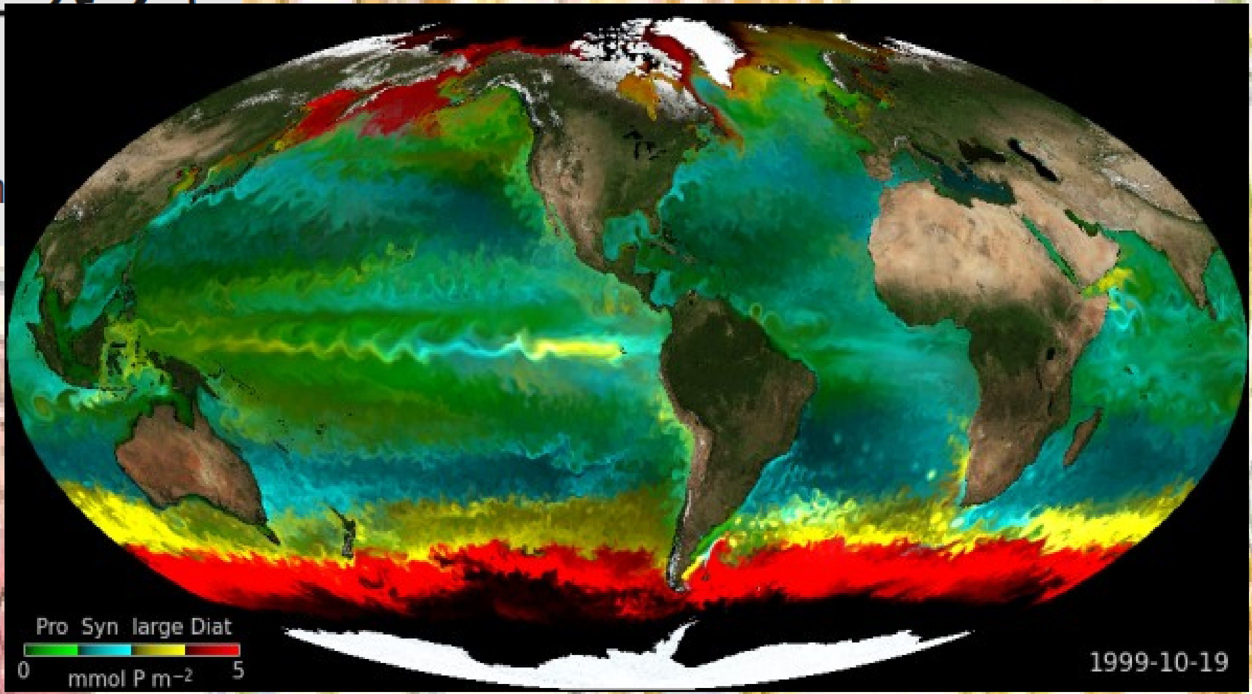
Modeling Marine Microbes: Past, Present and Prospects

Mick Follows
MIT

$$\frac{dP}{dt} = P(\mu - K - gZ)$$





What do we mean by models?

- Concepts
- Statistical relationships
- Mathematical descriptions
- Numerical models

Why theory and numerical models?

- Formalize and synthesize conceptual understanding
- Explore how a complex system operates
- Quantitative applications
  - Data interpolation and state estimation
  - Prediction
  - weather forecasting

Outline

- First models of marine plankton populations
- Numerical models
- Functional diversity – JGOFS era
- Diverse, self-assembling model communities
- Genomic era
- Physiological parameterizations
- What next?

Fleming (1939)

Modeled spring bloom as predator-prey system

214 Richard H. Fleming

$$\frac{dP}{dt} = \mu P - g(t)$$

growth grazing

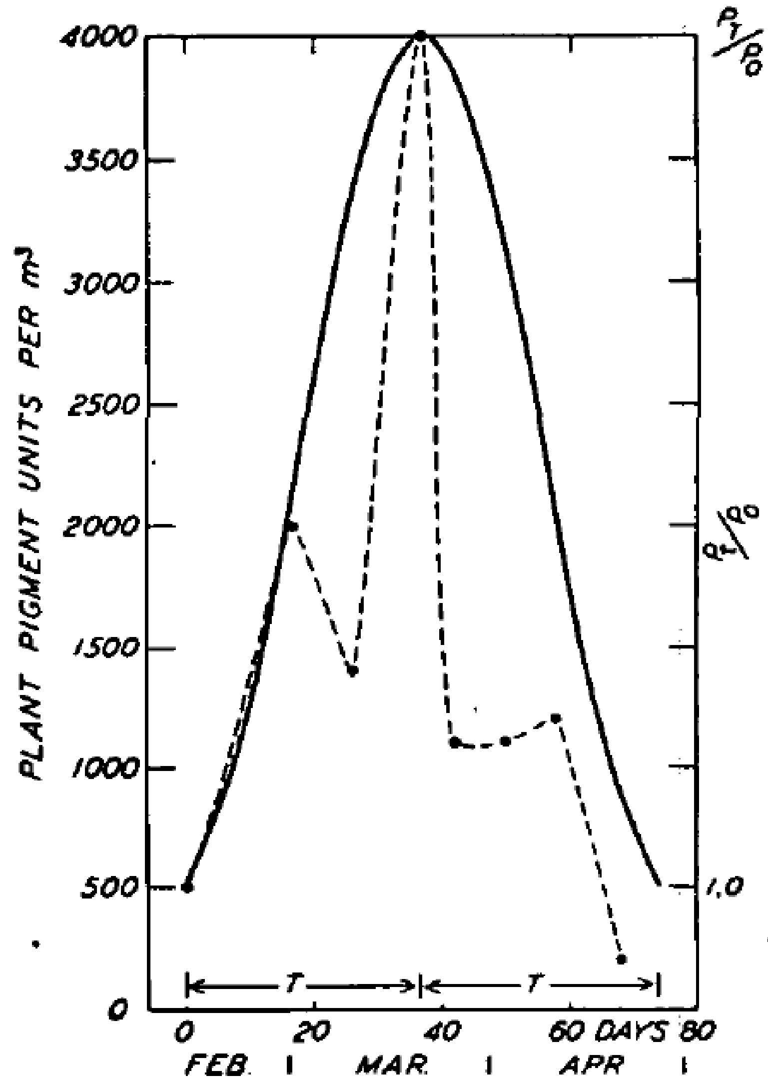


Fig. 1. Heavy line indicates the computed population curve for the spring diatom maximum observed by Harvey *et al.* in the English Channel in 1934. Broken line joins the points of observation. The computed curve was fitted to the initial and maximum populations.

Riley (1946): Modeled seasonal cycle of phytoplankton at Georges Bank

$$\frac{dP}{dt} = P(\mu - K - gZ)$$

rate of change   growth   respiration   grazing

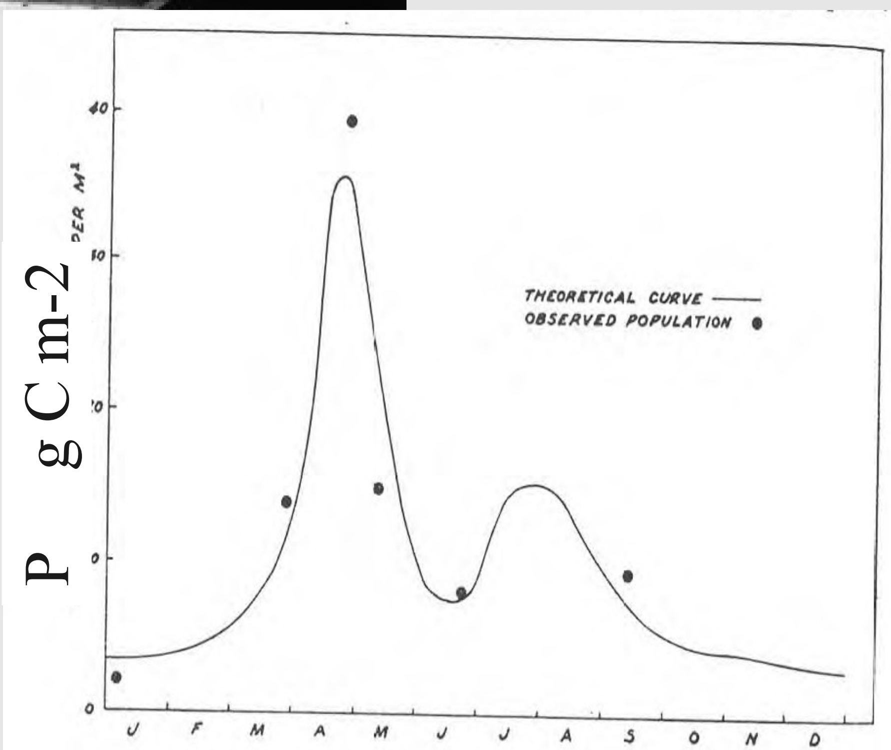


Figure 21. Curve shows the calc[...] cycle of phytoplankton, determined by approximate integration of the equ[...]te of change of the population. For comparison the observed quantities [...] are shown as dots.

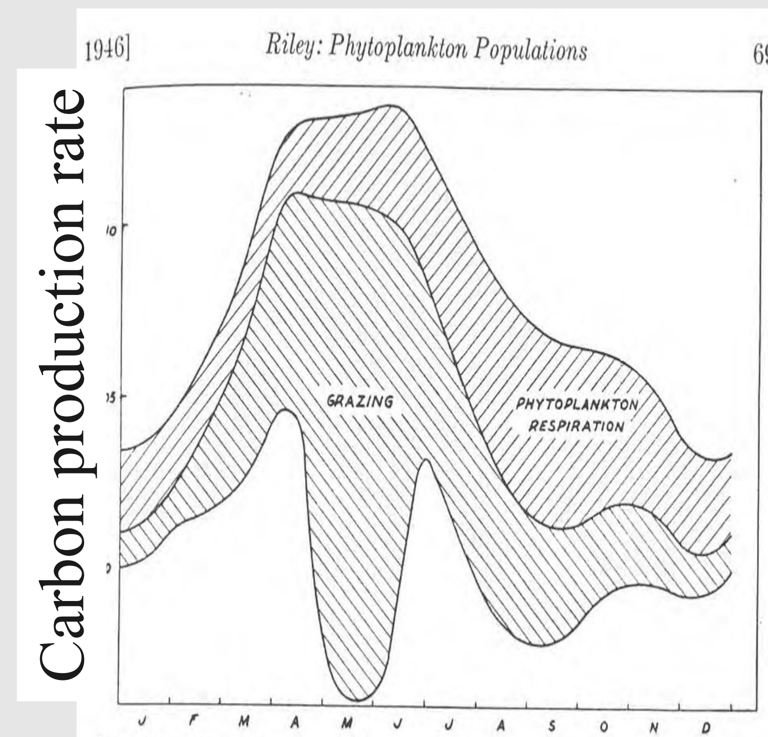
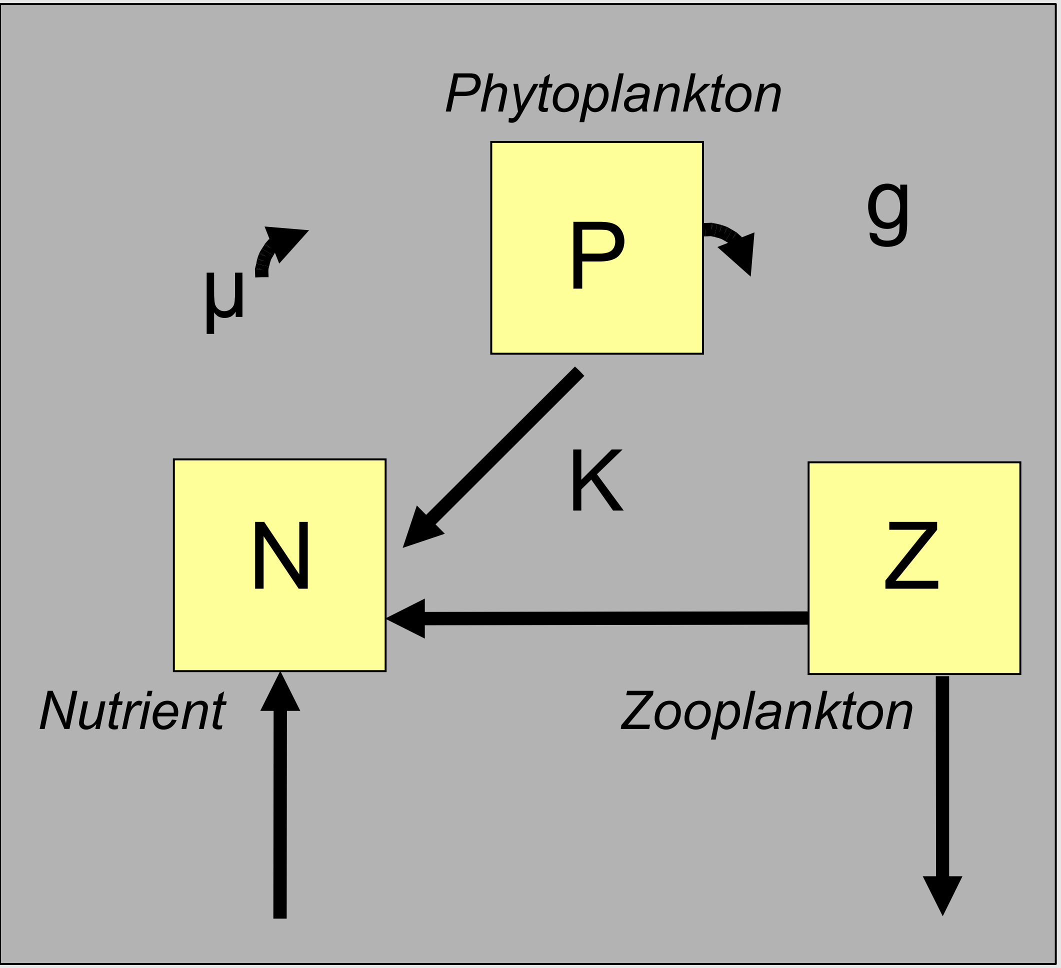


Figure 20. Estimated rates o[...]nsumption of carbon. Curve at top is the photosynthetic rate. By su[...]tory rate the second curve is obtained, which is the phytoplankton pr[...]n this is subtracted the zooplankton grazing rate, yielding the curve a[...] bottom, which is the estimated rate of change of the phytoplankton.

Steele (1958) NPZ models



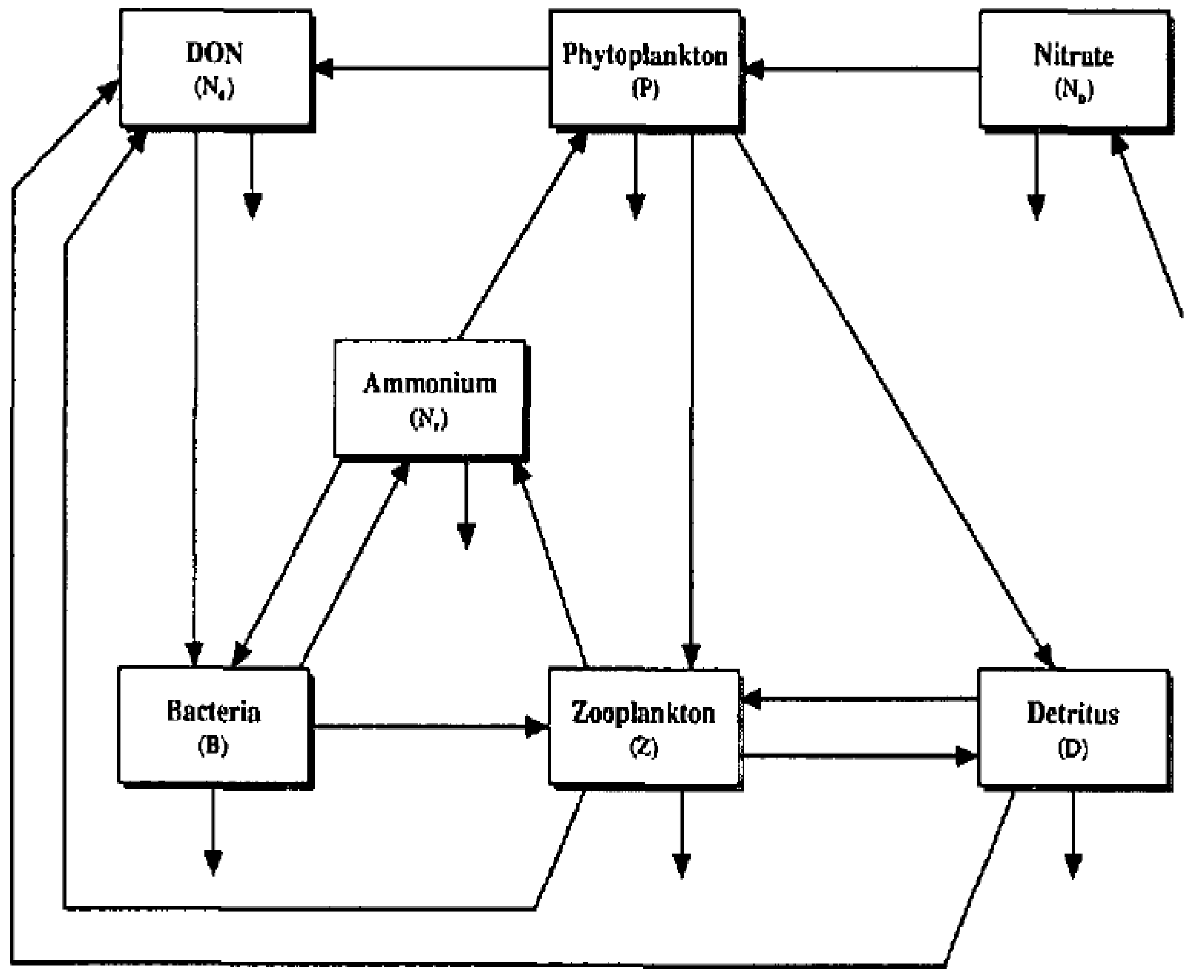
- Coupling *nutrient*, *autotroph*, and *herbivore* dynamics
- Enforce conservation of nutrient elements
- ***Numerical solutions*** with computers allowed sensitivity studies

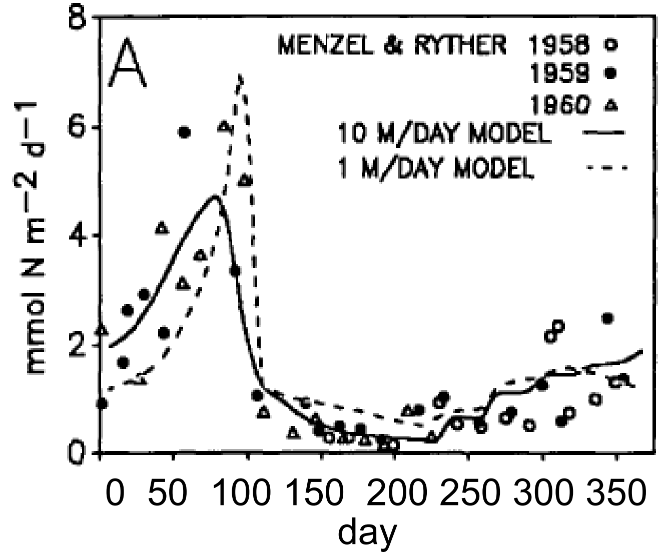
$$\frac{dN}{dt} = -\mu NP + KP + m(No - N)$$

$$\frac{dP}{dt} = P(\mu N - K - gZ - m)$$

$$\frac{dZ}{dt} = gZ - MZ^2$$

Fasham et al (1990): "Open Source" model





Numerical models of atmospheric and oceanic circulation

L.F. Richardson – early 20th century

Equations of fluid motion

Conservation of mass and momentum

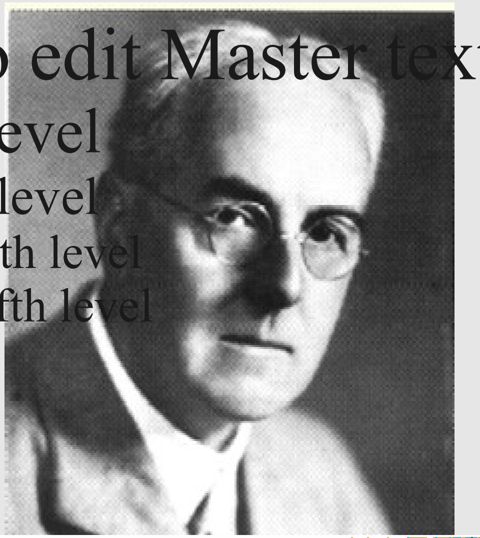
discretize world into a grid

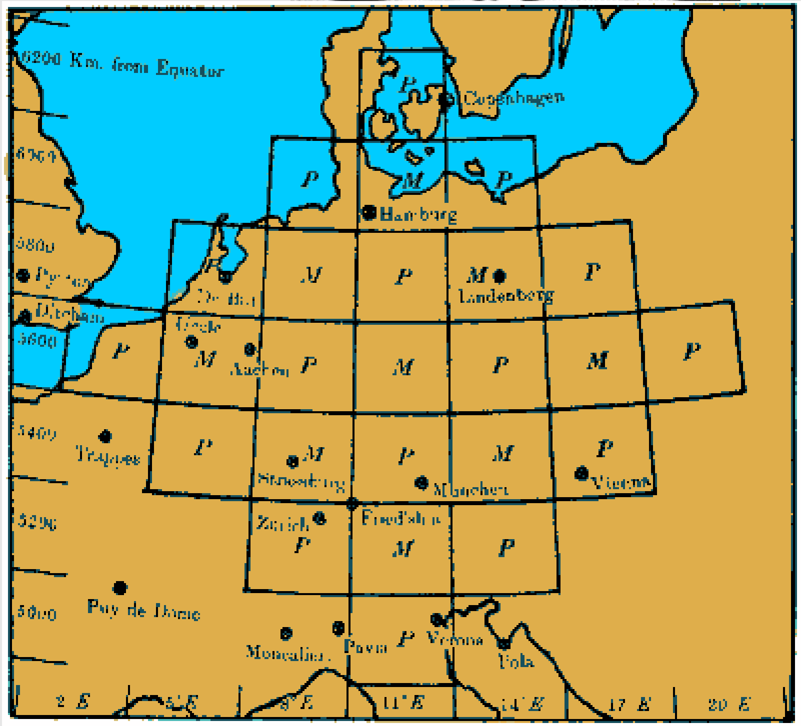
calculate how properties are transported from one grid cell into another

Move forward over a short time interval

Repeat…

Click to edit Master text sty
Second level
- Third level
  - Fourth level
    - Fifth level





Numerical models of ocean circulation

Motion

$$\frac{\partial \mathbf{v}_h}{\partial t} = \mathbf{G}_{v_h} - \nabla_h p$$

$$\frac{\partial w}{\partial t} = G_w - \frac{\partial p}{\partial z}$$

Continuity

$$\nabla \cdot \mathbf{v} = 0$$

Heat

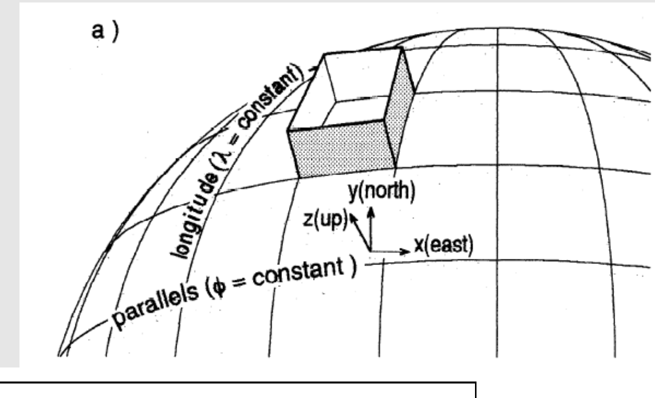
$$\frac{\partial T}{\partial t} = G_T$$

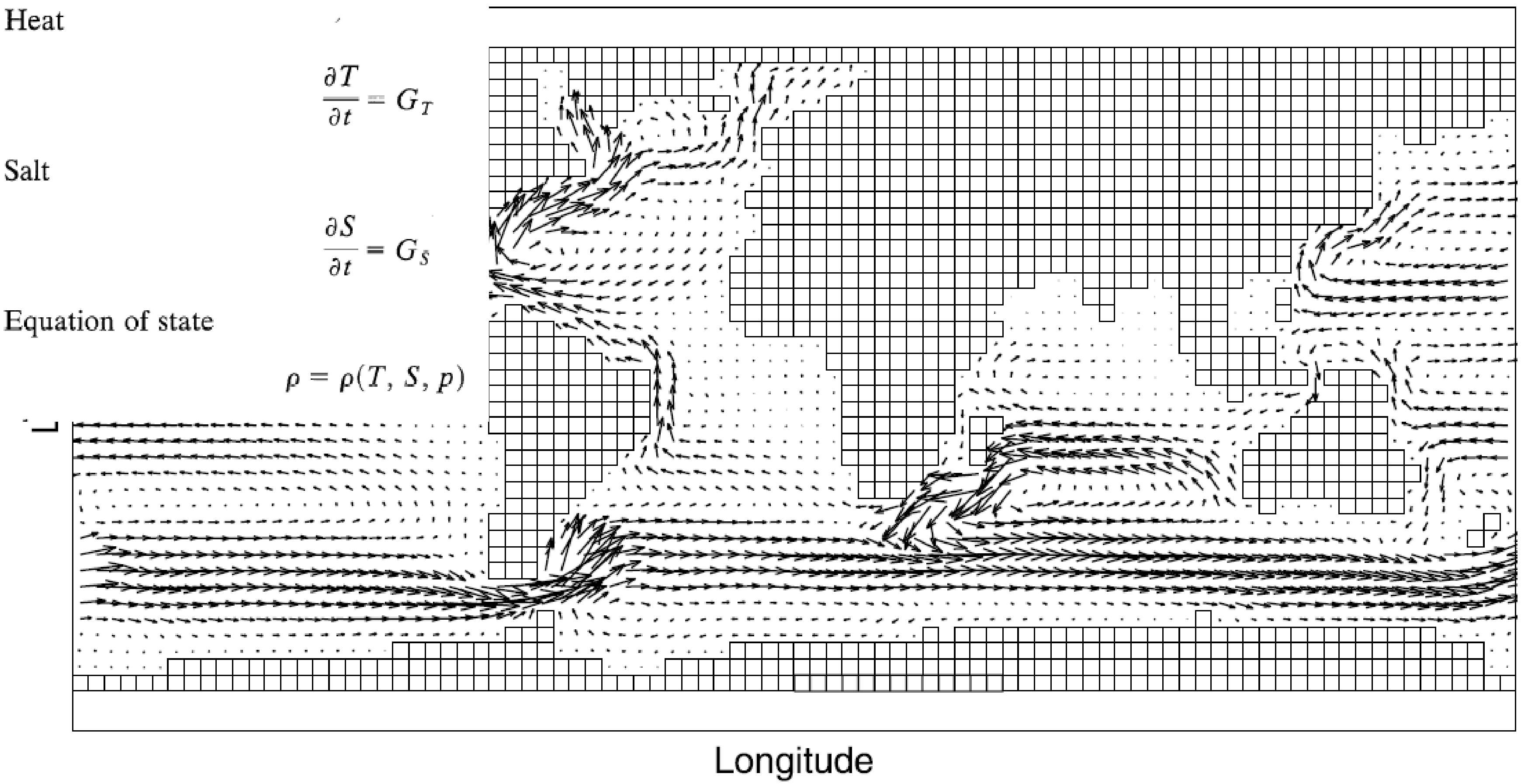
Salt

$$\frac{\partial S}{\partial t} = G_S$$

Equation of state

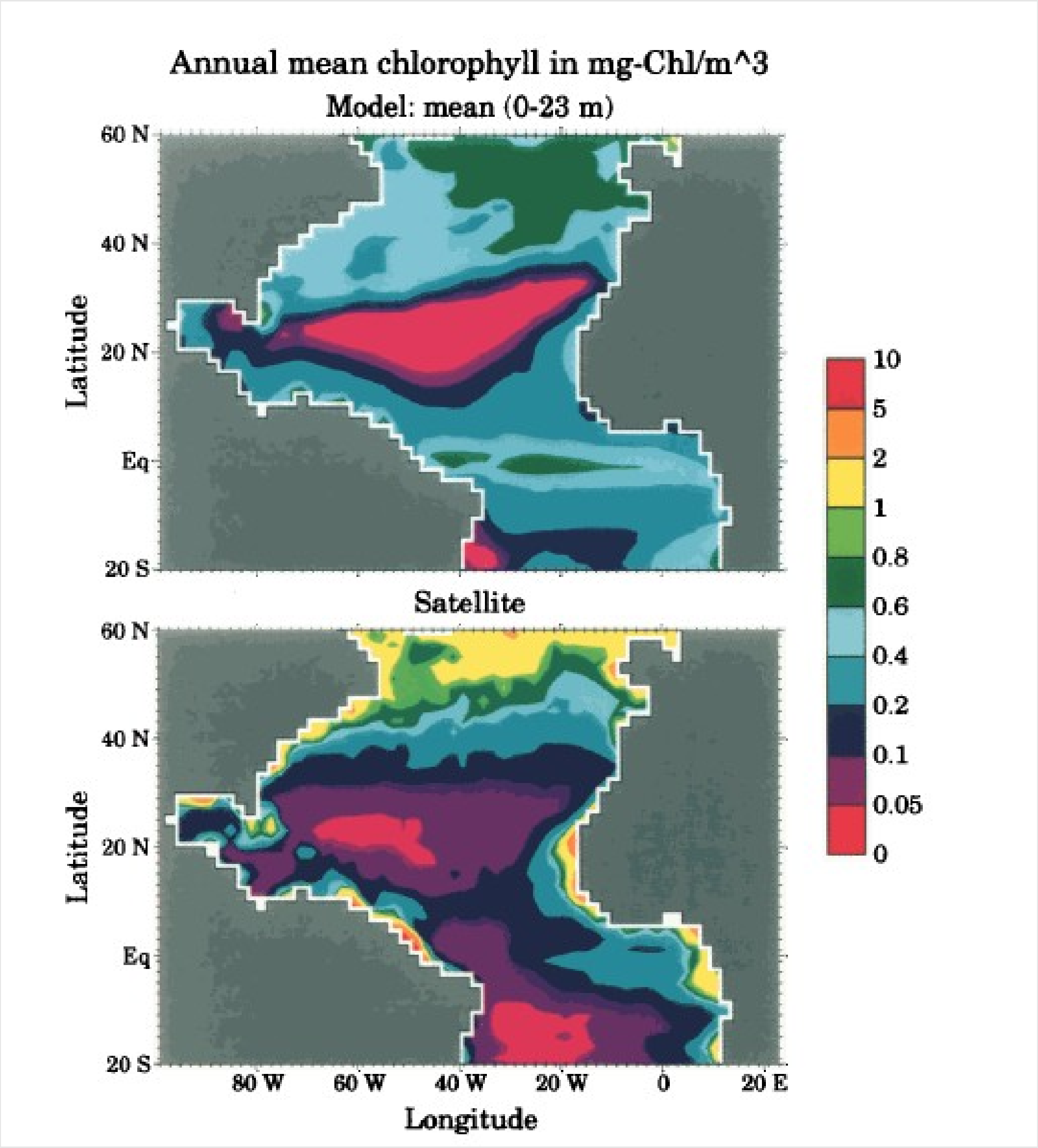
$$\rho = \rho(T, S, p)$$





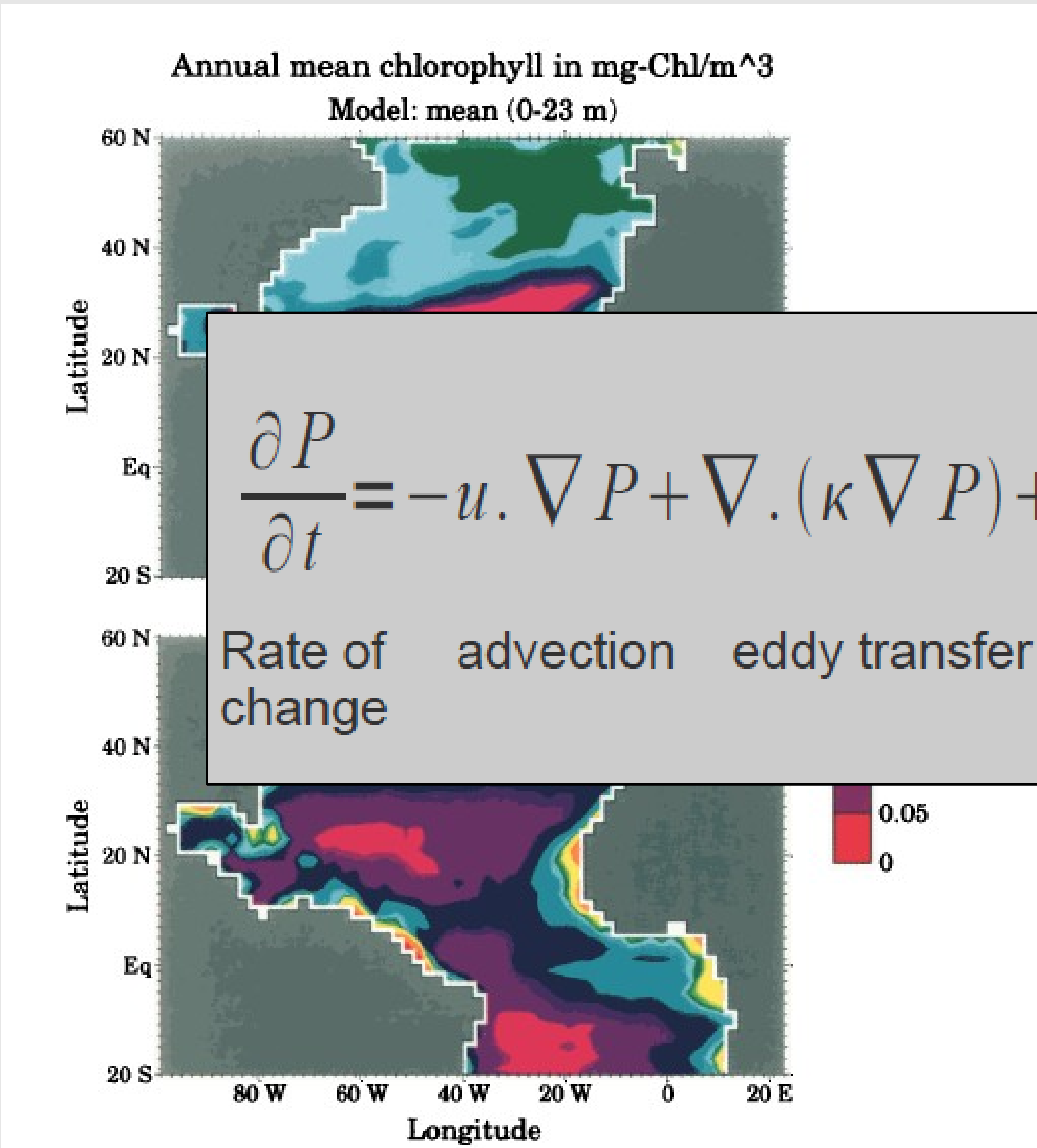
Currents at 450m

Sarmiento, Fasham et al (1993)



- Fasham, Ducklow & McElvie ecosystem model coupled to 3D North Atlantic circulation model
- Detailed analysis of budgets and fluxes
- Address in situ and remote data sets
- Evaluate role of physical transport processes for nitrate

Sarmiento, Fasham et al (1993)



- Fasham, Ducklow & McElvie model in 3D North Atlantic

$$\frac{\partial P}{\partial t} = -u.\nabla P + \nabla.(\kappa \nabla P) + \mu(I, N_x, T)P - gZf(P) + \ldots$$

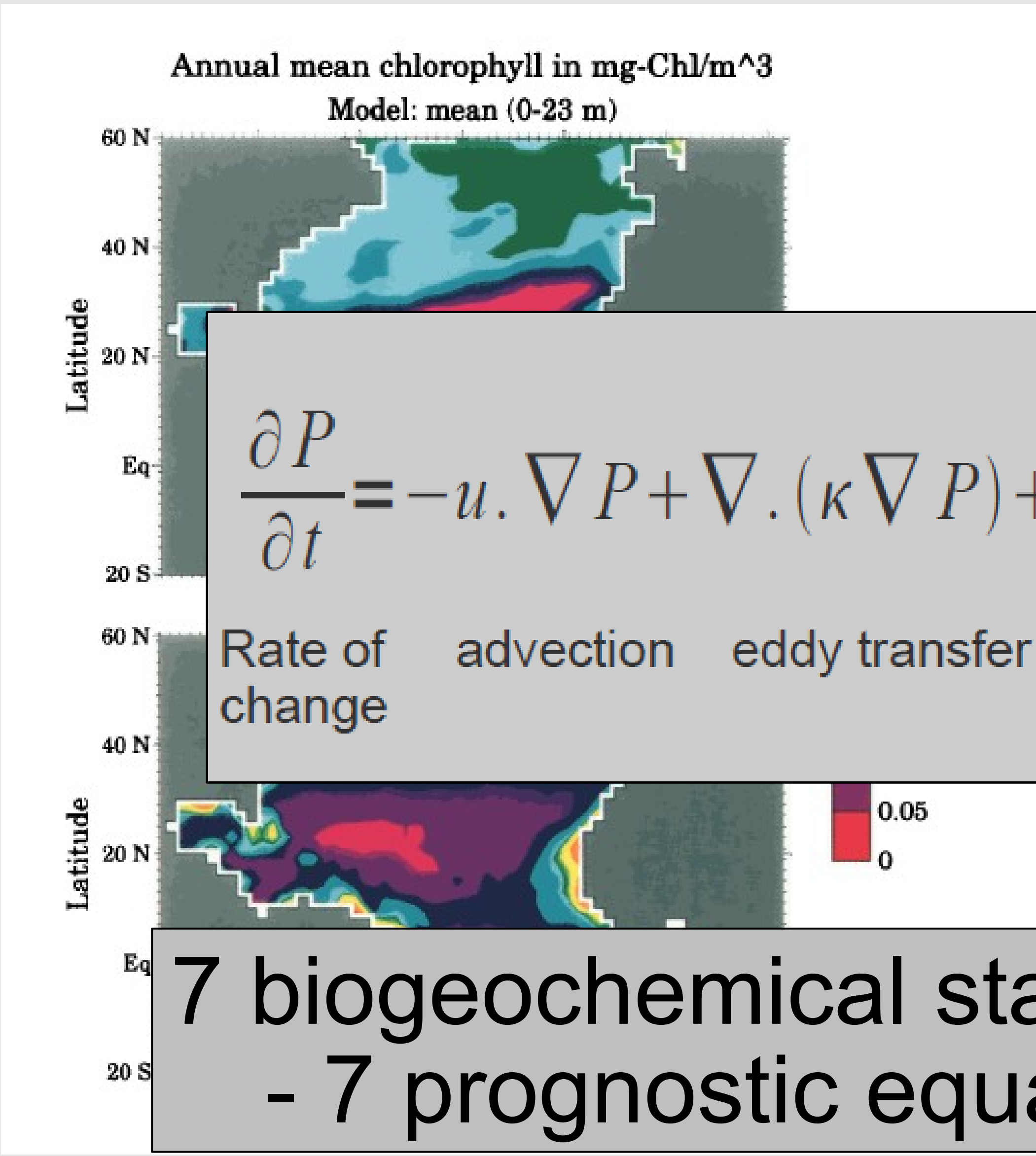
Rate of change | advection | eddy transfer | growth | grazing | ...

f

remote data sets

- Evaluate role of physical transport processes for nitrate

Sarmiento, Fasham et al (1993)



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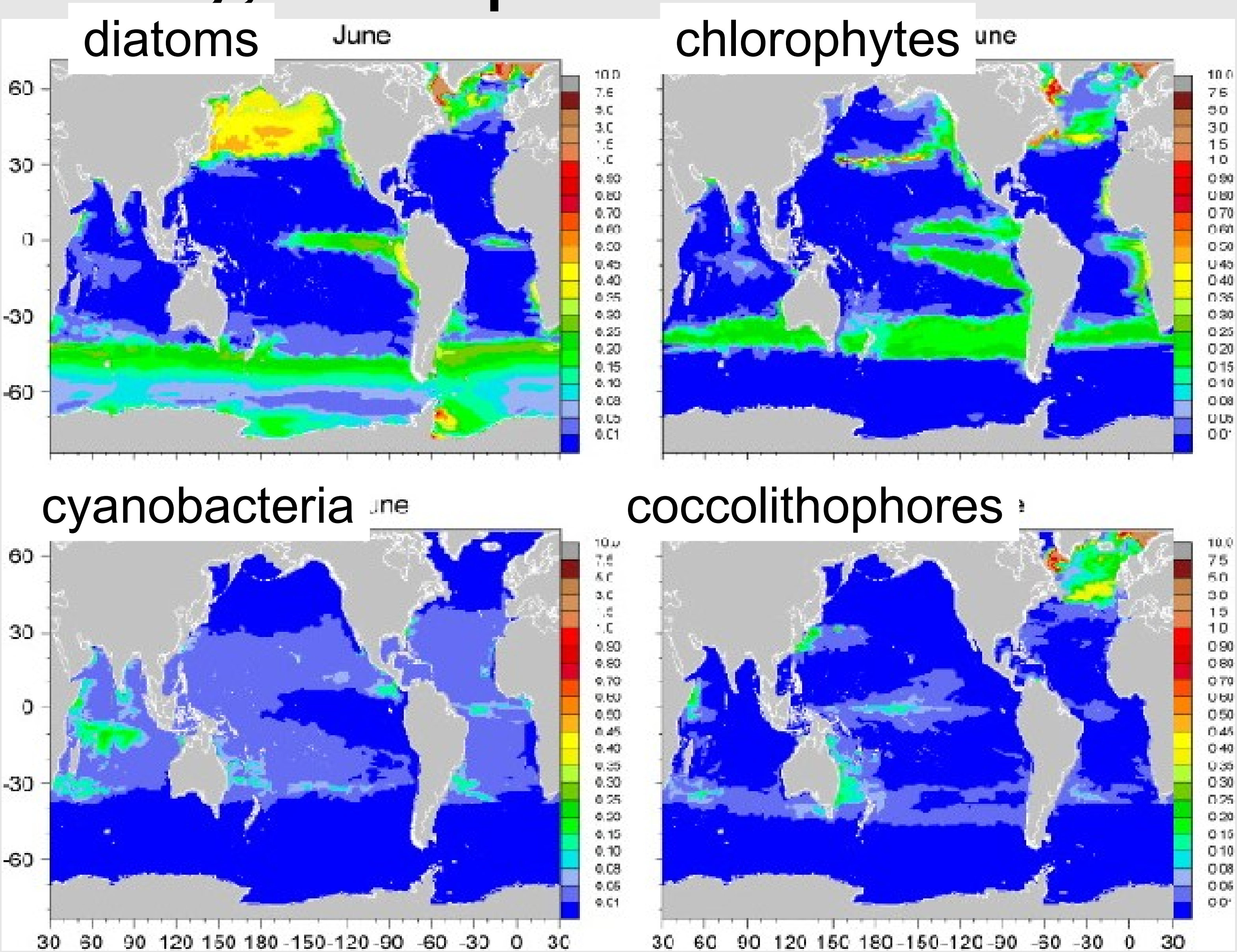
Rate of change | advection | eddy transfer | growth | grazing | ...

- Evaluate role of ...nsport ...or nitrate

7 biogeochemical state variables;
 - 7 prognostic equations

JGOFS era:Resolving functional diversity, multiple nutrient elements



Gregg and Casey (2007)

Differentiation of functional groups

- Prescence/absence of functional ability
- Values of basic parameters which set rates/efficiencies for each organism type

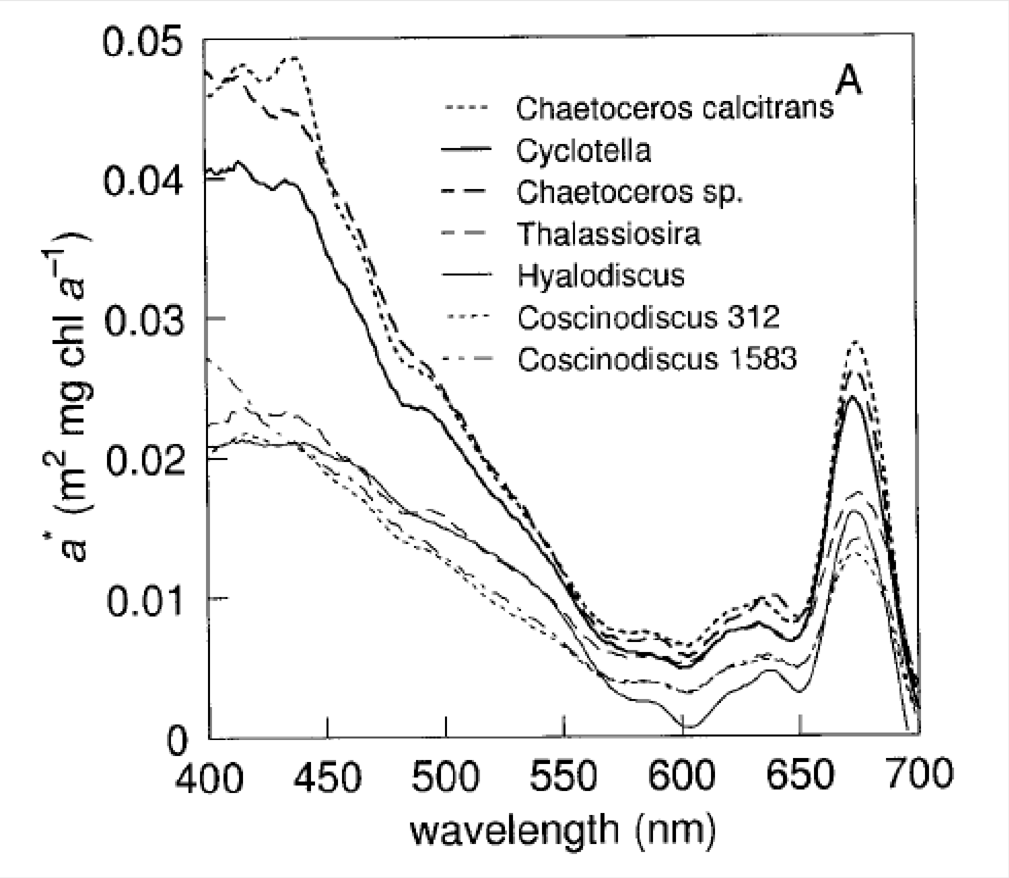
$$\frac{DP_1}{Dt} = P_1(\mu_1 - K_1 - g_{1Z})$$

$$\frac{DP_2}{Dt} = P_2(\mu_2 - K_2 - g_{2Z})$$

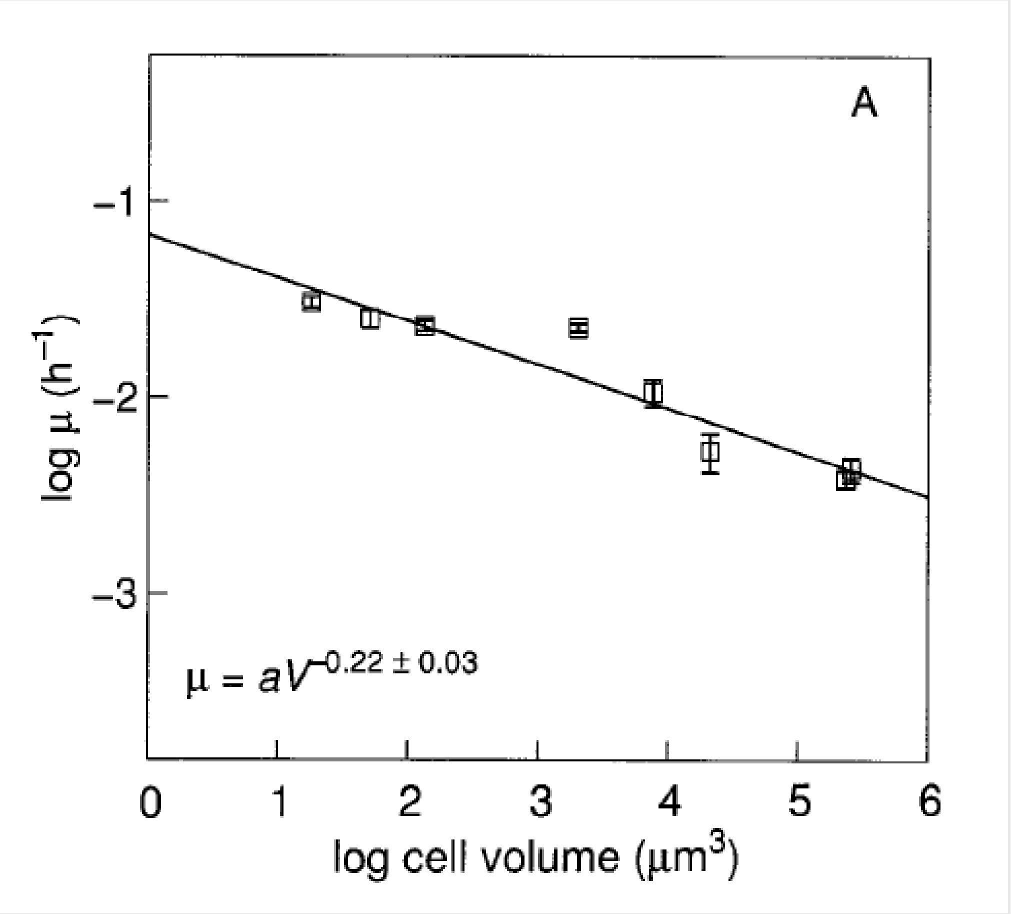
How to define functional groups: e.g. What is an "average" diatom?

- Allometric, phenotypic and genotypic variety

light absorbtion

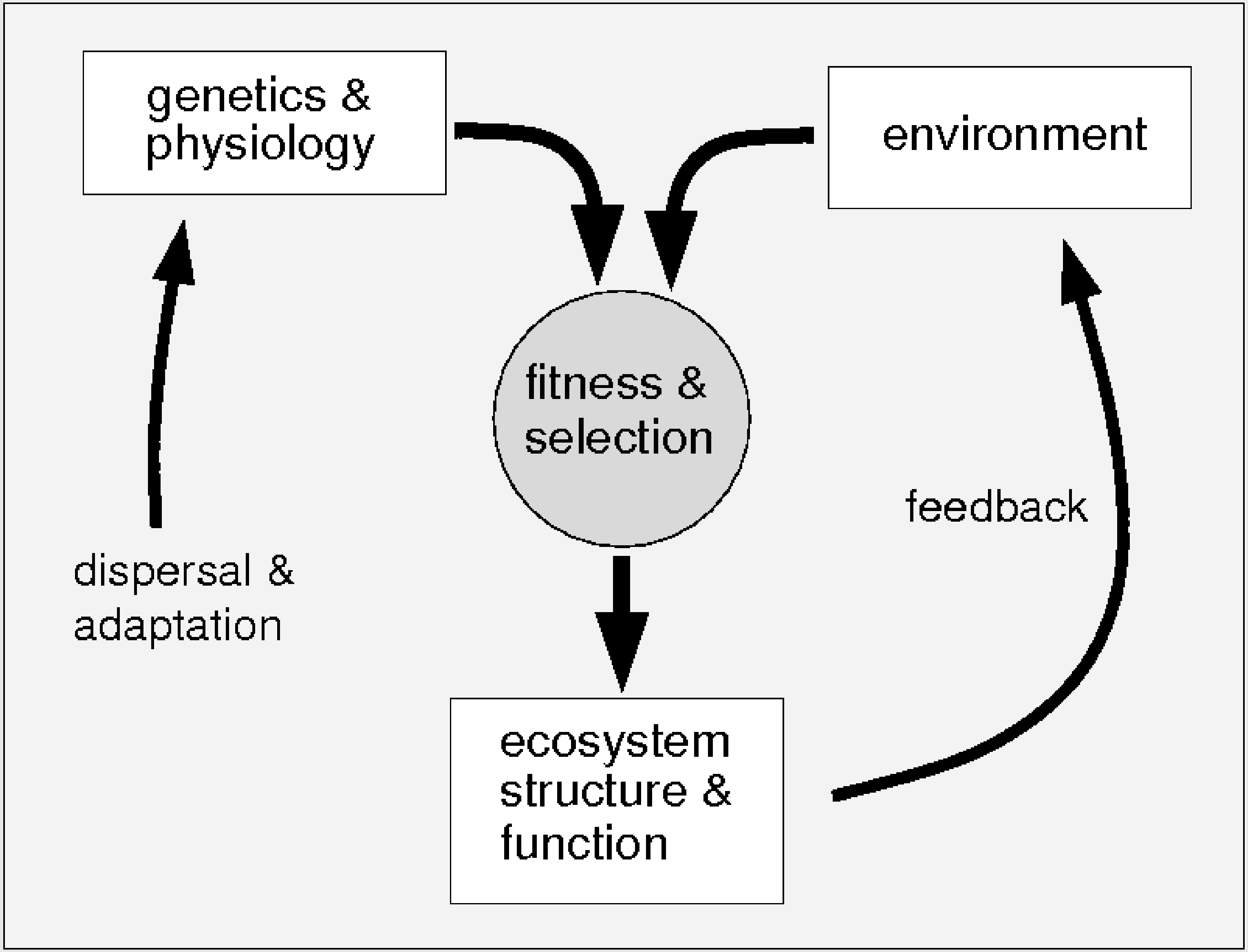


growth rate



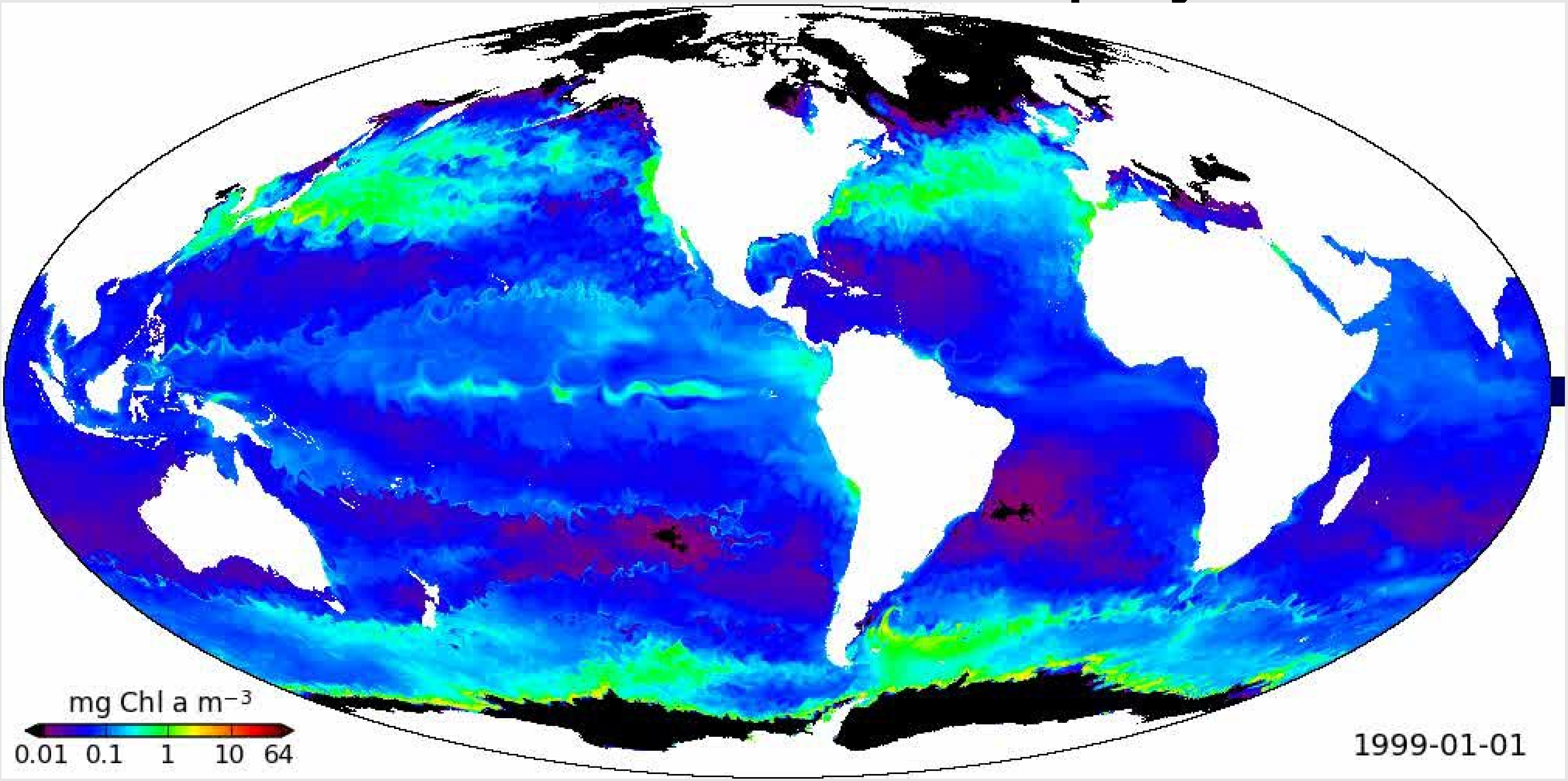
Zoe Finkel (2001)

Self-assembly of marine microbial communities



verything is everywhere but the environment selects" - Baas Becking (1934)

Modeled surface Chlorophyll 1999



MIT ocean circulation model,

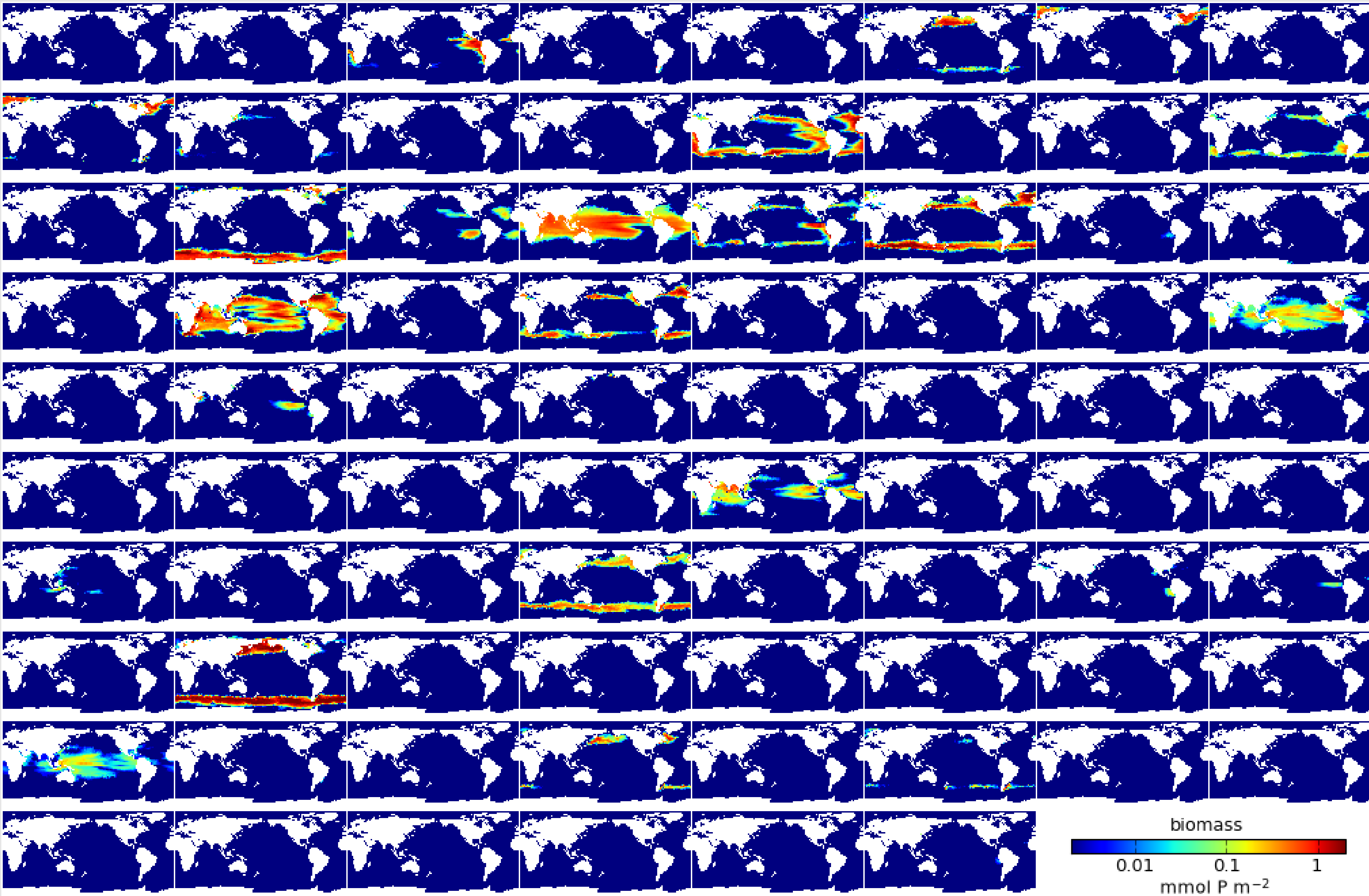
cycles of N,P,Si, Fe,

seeded with ~100 phytoplankton phenotypes

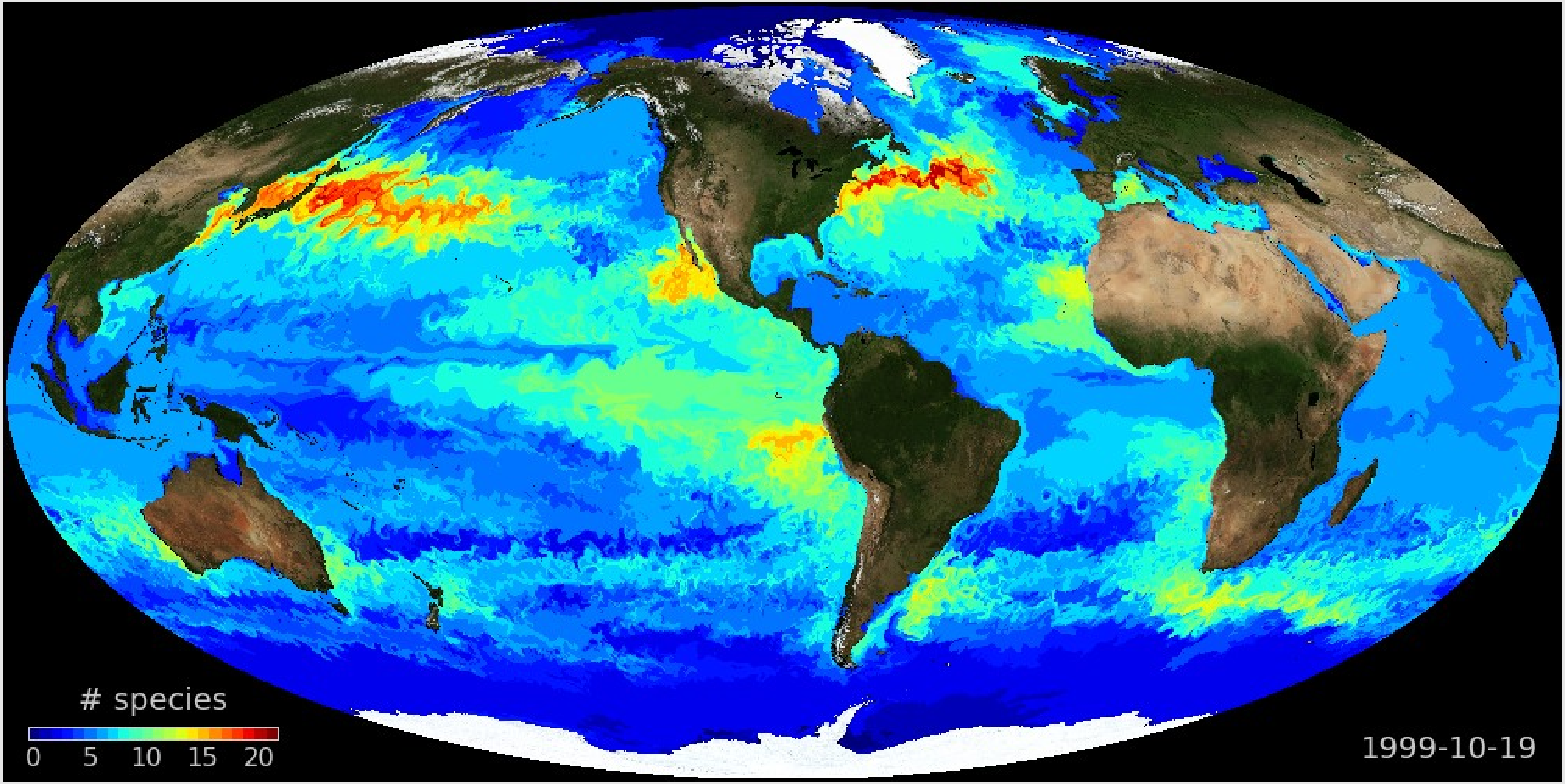
2 types of grazer...

Oliver Jahn, Stephanie Dutkiewics, Chris Hill, Jason Bragg

Contributions from many 10's of model "species"

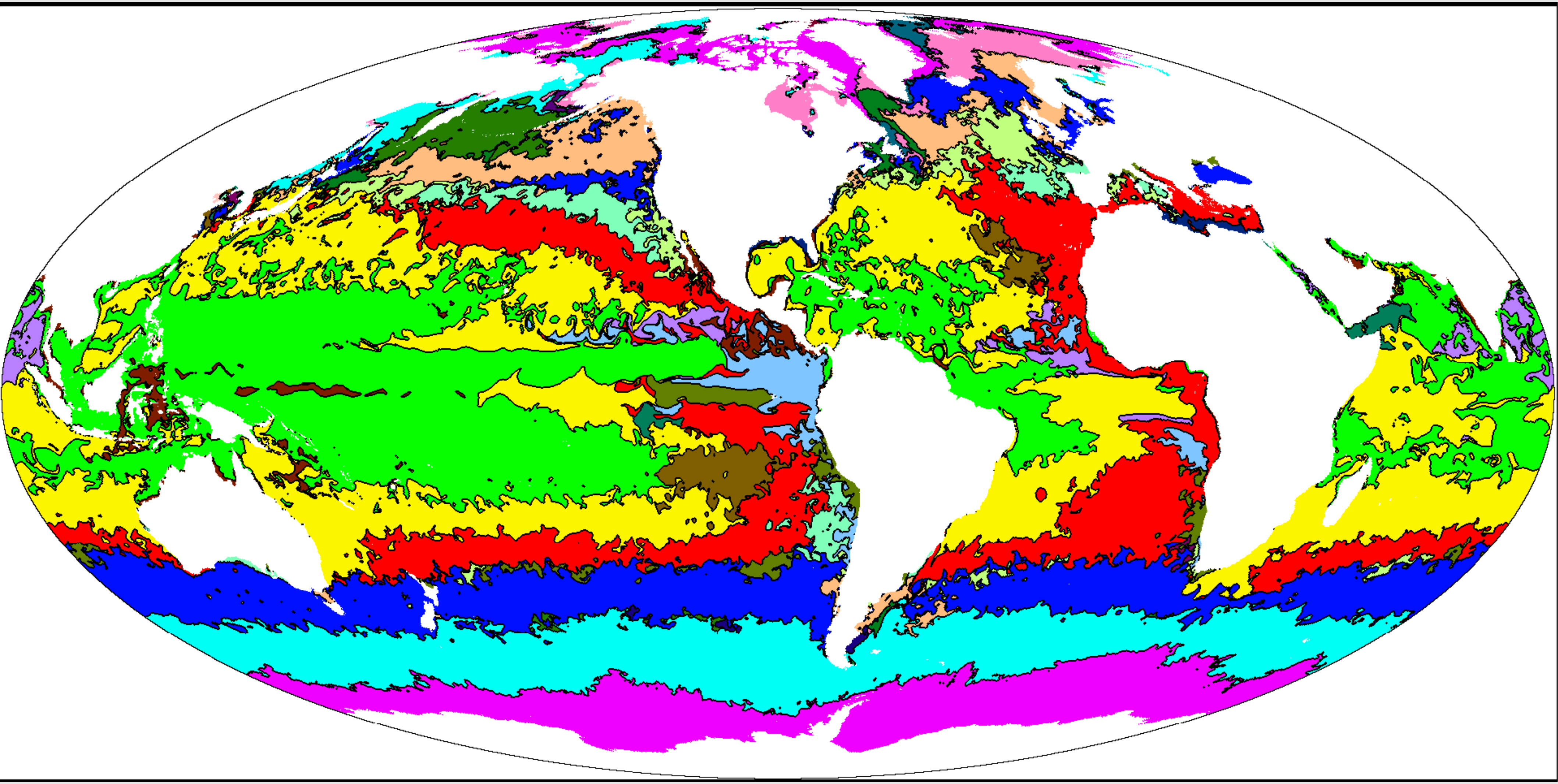


“Biodiversity” of modeled phytoplankton population



Barton et al (2010)

Model's biogeographical provinces based on changes in "species" assemblages



c.f. Longhurst

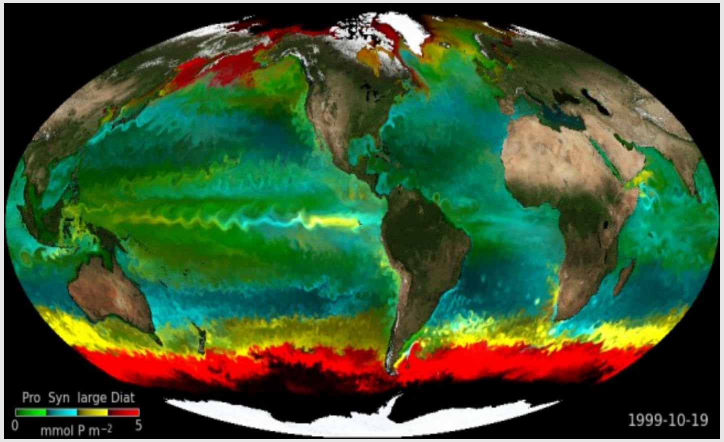
Biogeography: Niche differentiation

Computational cost

$$\frac{\partial P}{\partial t} = -u.\nabla P + \nabla.(\kappa \nabla P) + \mu(I, N_x, T)P - gZf(P) + \ldots$$

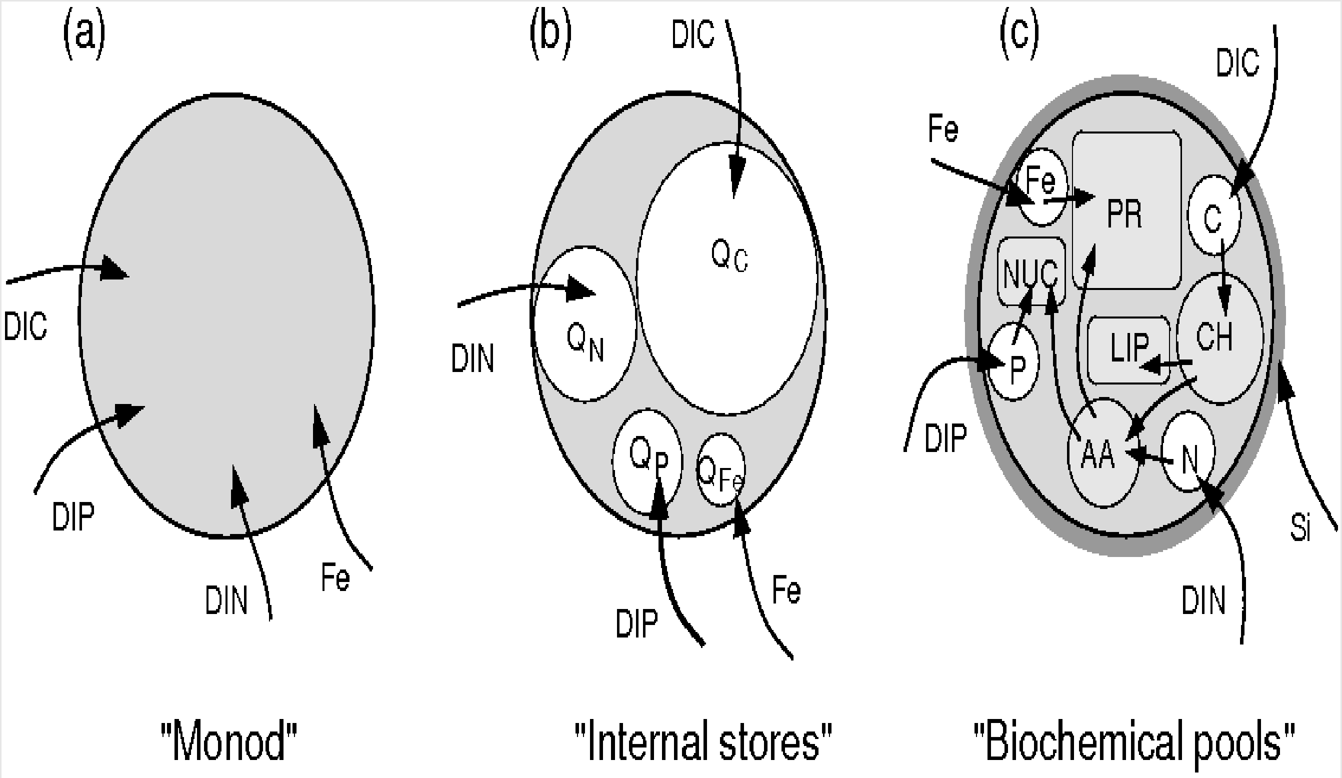
Rate of change	advection	eddy transfer	growth	grazing	...

- For high physical and ecological resolution >80% of CPU time is spent on transport
- Illustrated model carries100 tracers
- Each phytoplankton “phenotype” is one state variable or one tracer
- Can handle O(1000) tracers



Physiological parameterizations

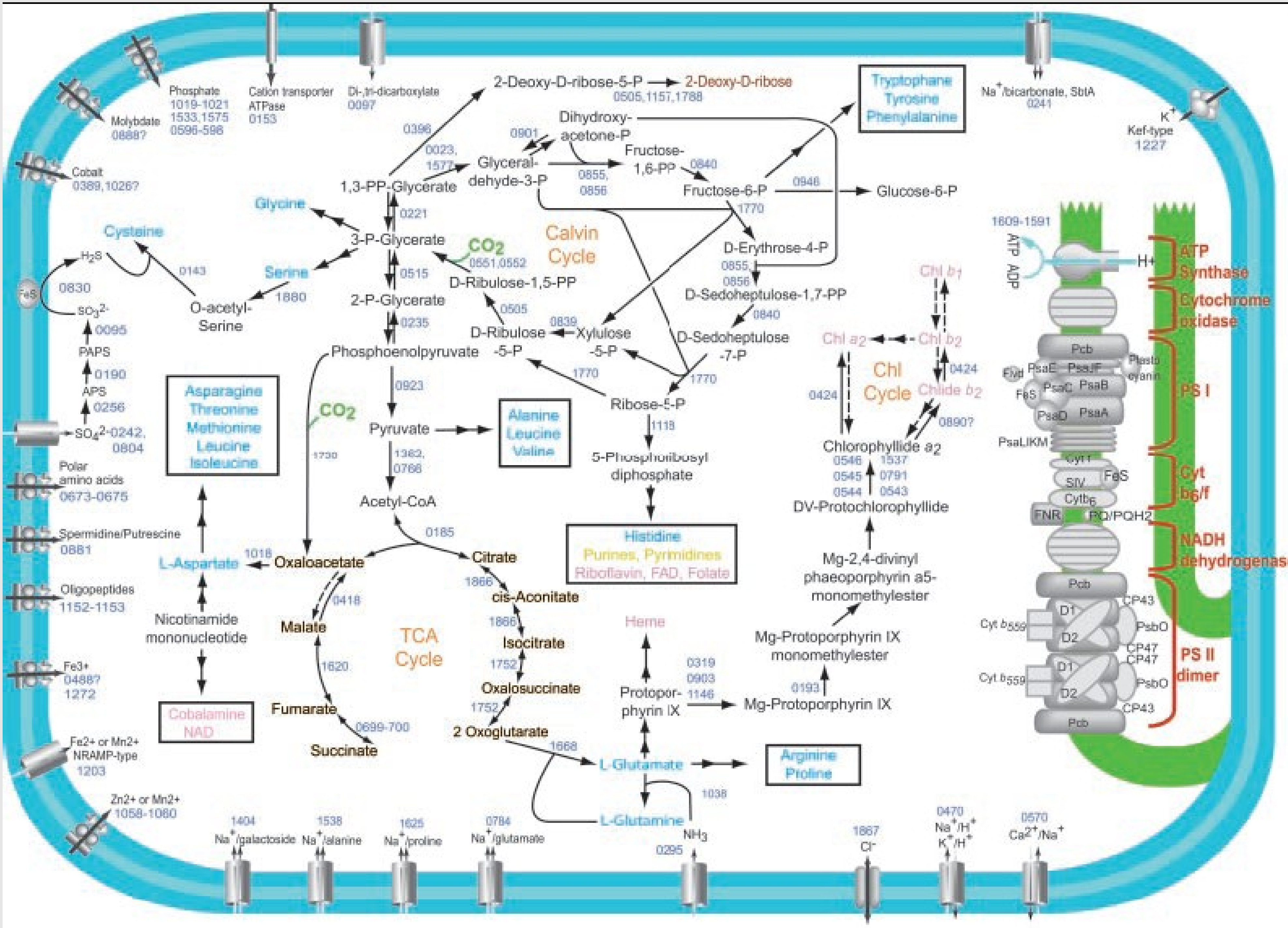
- Generally little change since Riley

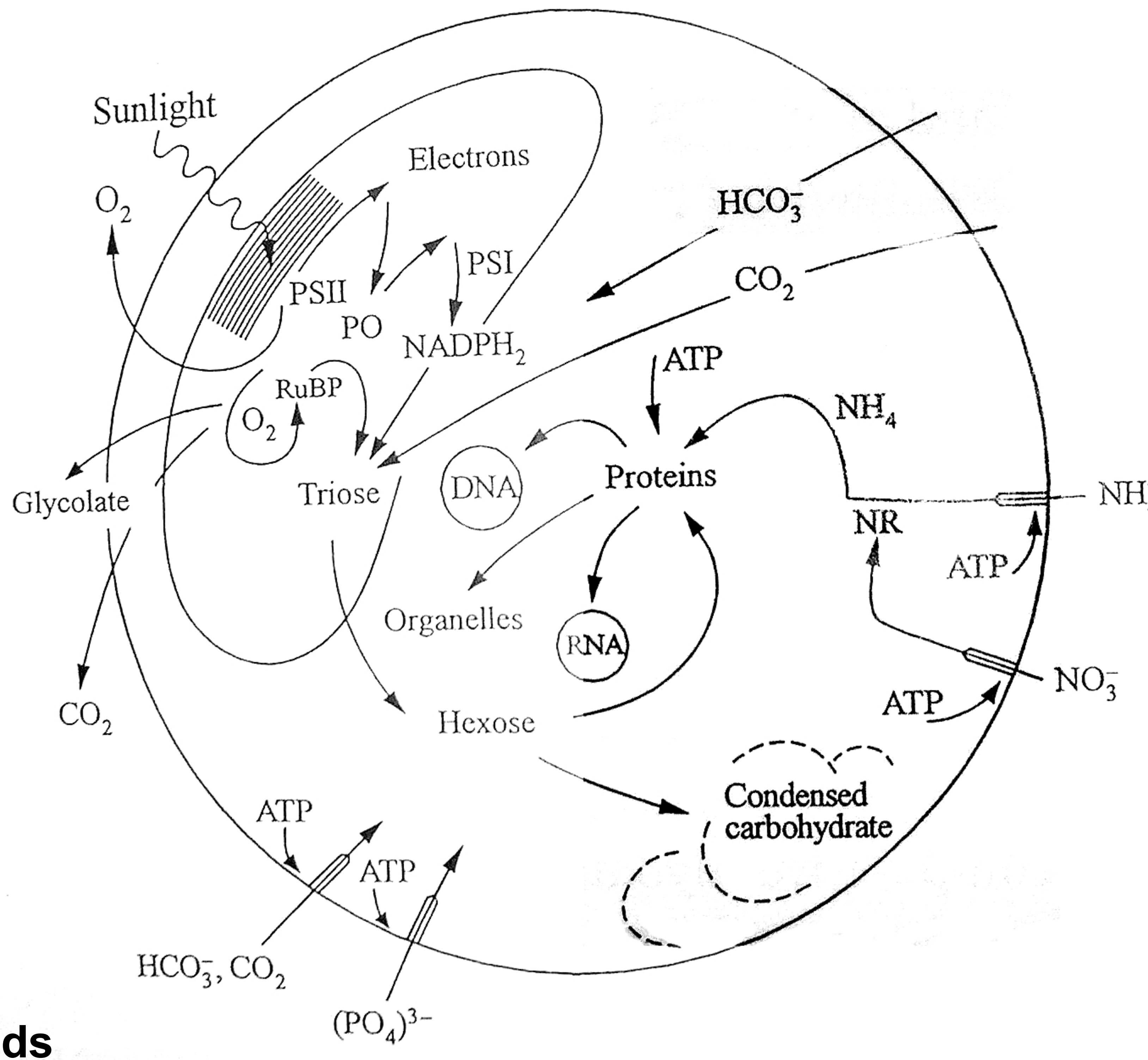


1 tracer per cell type
Fixed elemental ratios

Several tracers per cell type
1 per nutrient element
+ number density + Chl:C
Flexible elemental ratios

Metabolic pathways in *Prochlorococcus*
Dufresne et al. (2003)



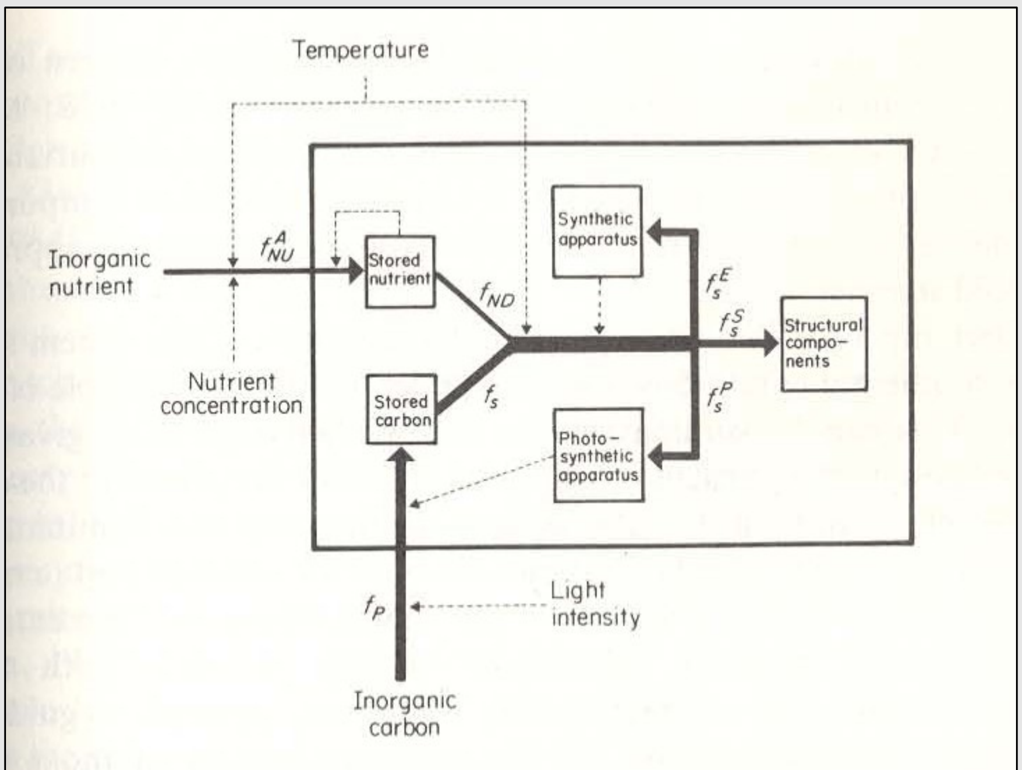


Sunlight
O_2
Electrons
PSII
PO
PSI
$NADPH_2$
HCO_3^-
CO_2
RuBP
O_2
Glycolate
Triose
DNA
Proteins
ATP
NH_4
NR
NH_4^+
ATP
Organelles
RNA
CO_2
Hexose
NO_3^-
ATP
Condensed carbohydrate
ATP
ATP
HCO_3^-, CO_2
$(PO_4)^{3-}$

Reynolds

1979: Physiological models of individual cells

Shuter – algal cell



Shuler et al. - *E. coli*

Shuler *et al.*: Mathematical Model for Growth of a Cell 37

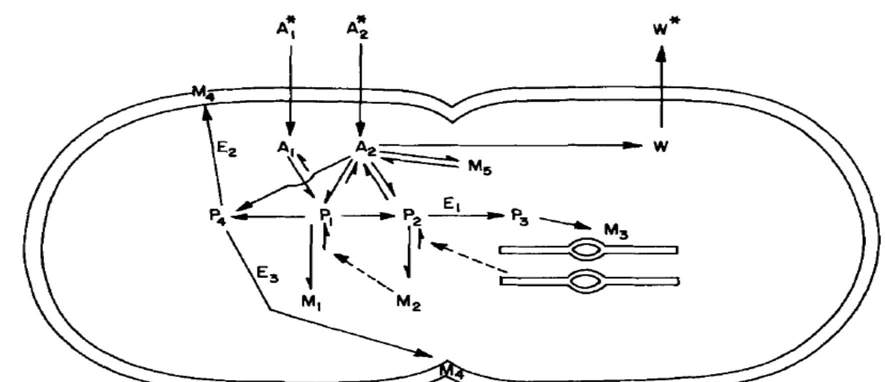
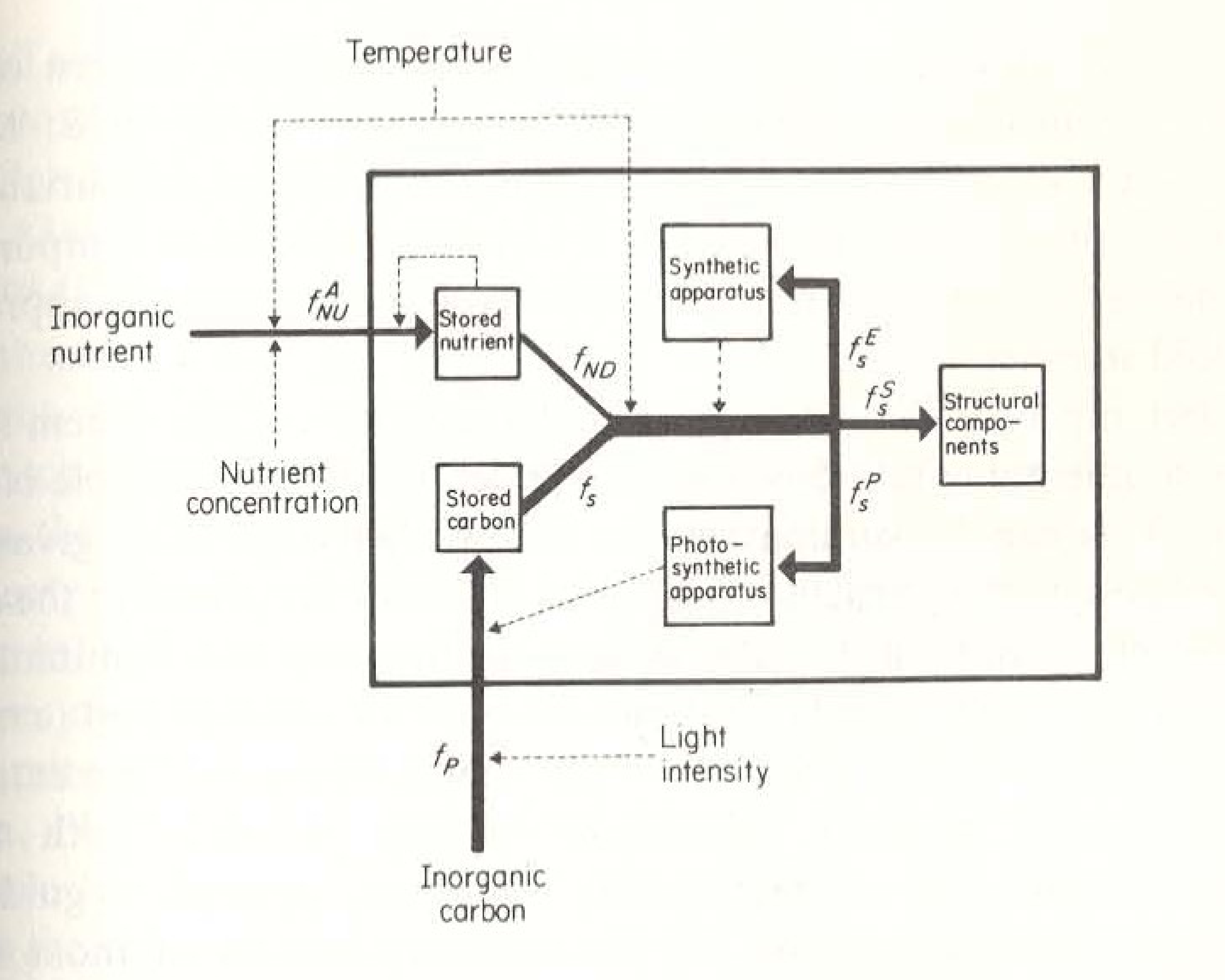


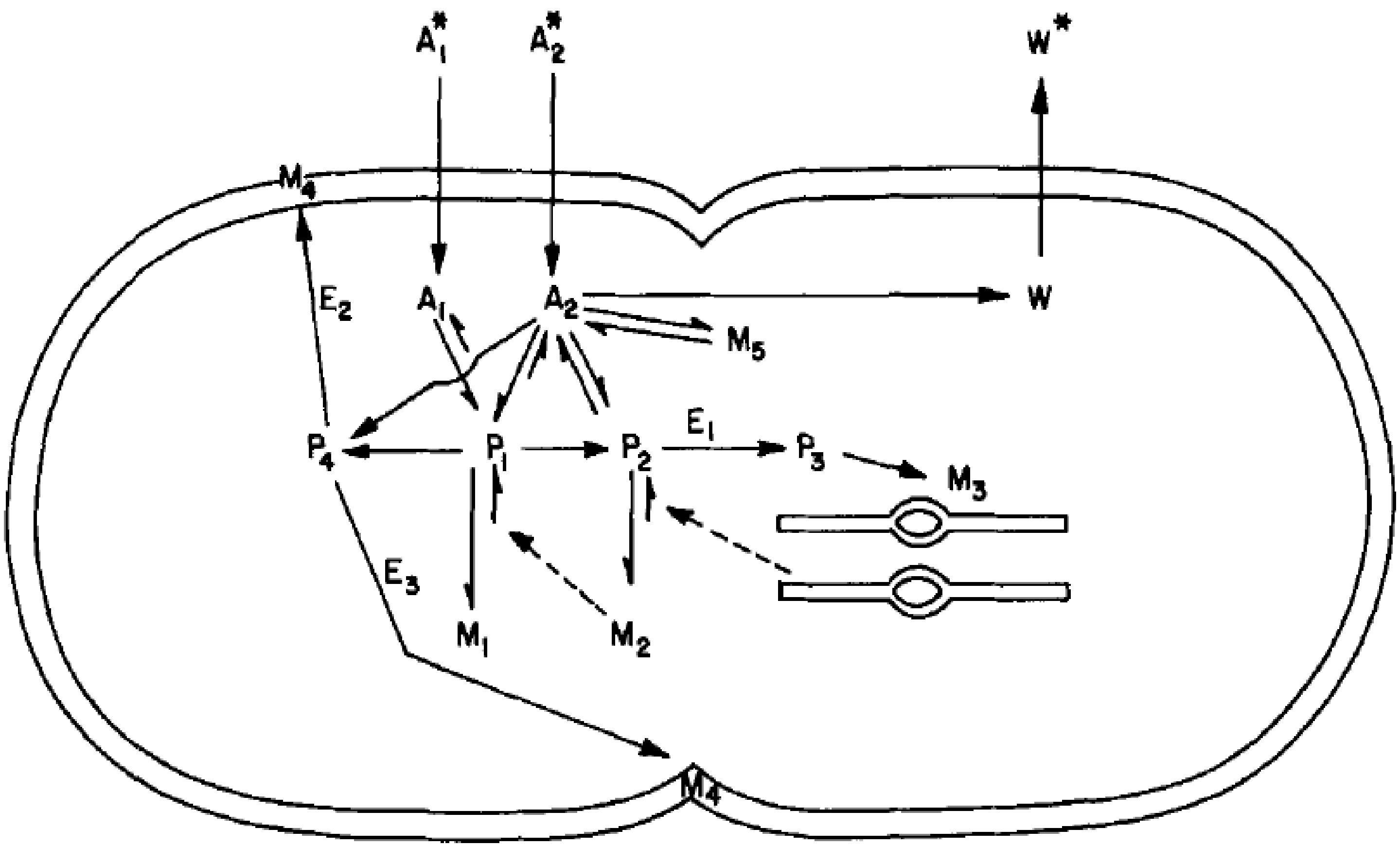
FIGURE 1. An idealized sketch of an *Escherichia coli* cell growing in a glucose-ammonium salts minimal medium is shown. At the time shown the cell has just completed a round of DNA replication and initiated septum (or cross-wall) formation and a new round of DNA replication. Solid lines indicate the flow of material; dashed lines indicate the flow of information. The symbols are defined below:

B., J Theor. Biol. 78, 519, (1979) Shuler et al., Annals NY Acad. Sci., (

Shuter (1979): A model of physiological adaptation in unicellular algae



Shuler et al (1979)



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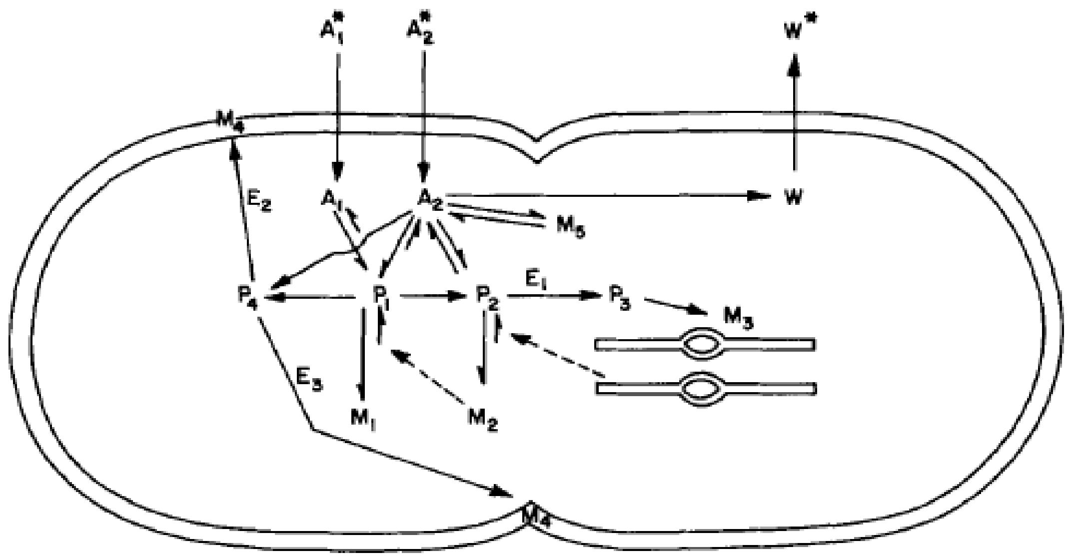

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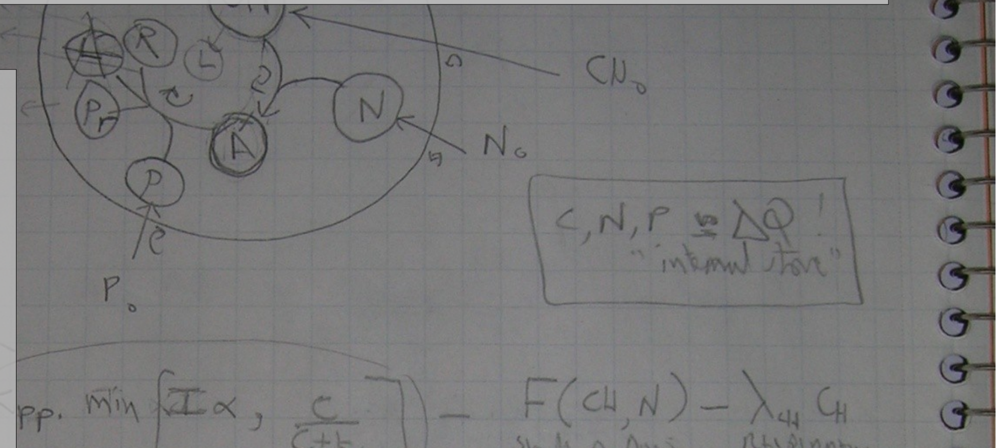
A_1 = ammonium ion
A_2 = glucose (and associated compounds in the cell)
W = waste products (as CO_2 & H_2O in aerobic growth) formed from energy metabolism
P_1 = amino acids
P_2 = ribonucleotides
P_3 = deoxyribonucleotides
P_4 = cell envelope precursors
M_1 = protein
M_2 = RNA
M_3 = DNA
M_4 = cell envelope including all membranes
M_5 = glycogen
E_1 = enzymes in the conversion of P_2 to P_3
E_2,E_3 = molecules involved in directing septum formation and cell envelope synthesis

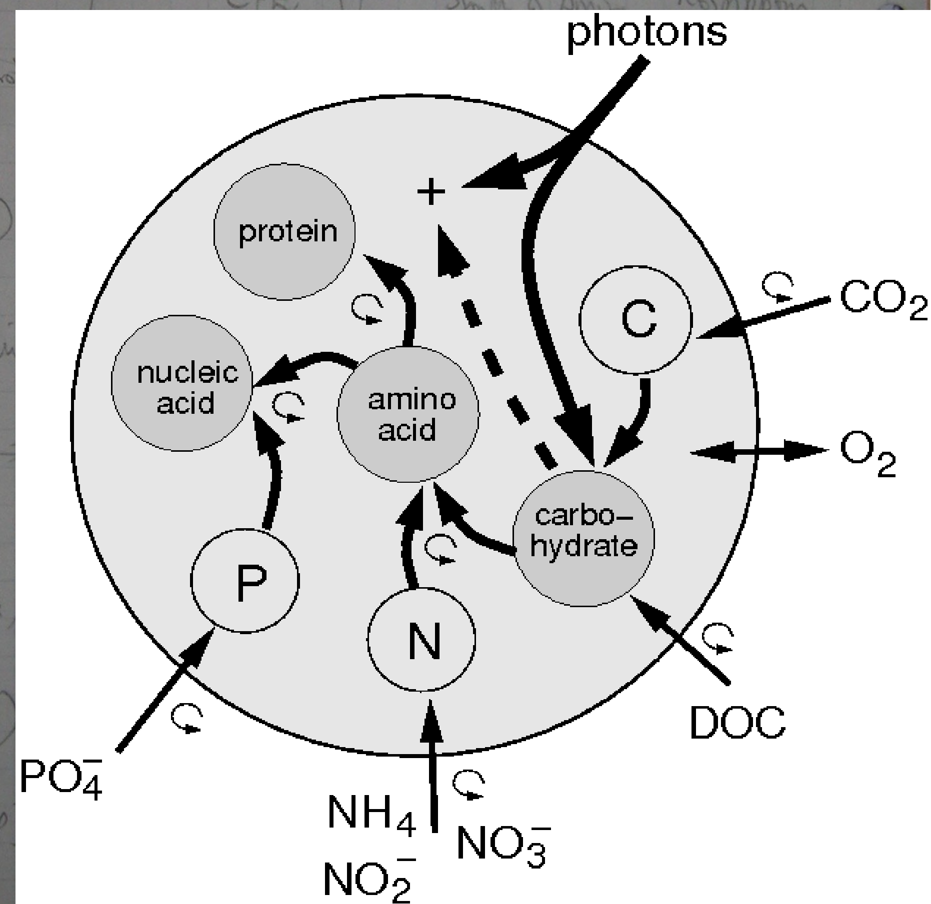
An * indicates that the material is present in the external environment.

Shuler et al (1979)

A biochemically motivated model?

- Individual-based form
- Can handle many millions of cells
- Re-cast in density form for ecological studies
- About 10 state variables per cell type
- c.f. internal stores model
- General model describes phototrophy and heterotrophy





“Virtual batch culture”

Number of cells

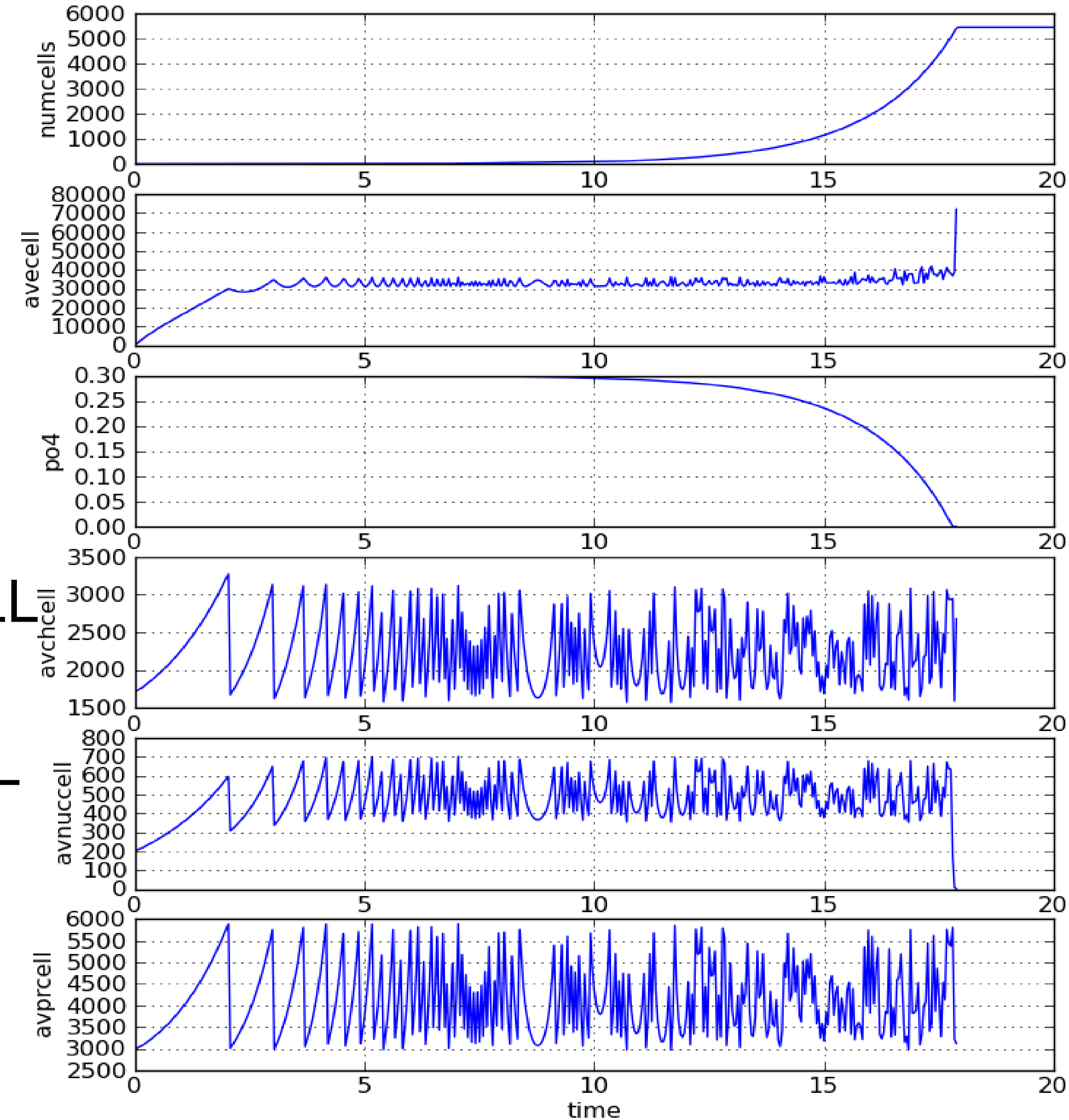
“ENERGY”/CELL

Phosphate in medium

“CARBOHYDRATE”/CELL

“NUCLEIC ACIDS”/CELL

“PROTEIN”/CELL



Biochemical fractionation of primary production by phytoplankton in Belgian coastal waters during short- and long-term incubations with ^{14}C-bicarbonate

I. Mixed diatom population

C. Lancelot and S. Mathot

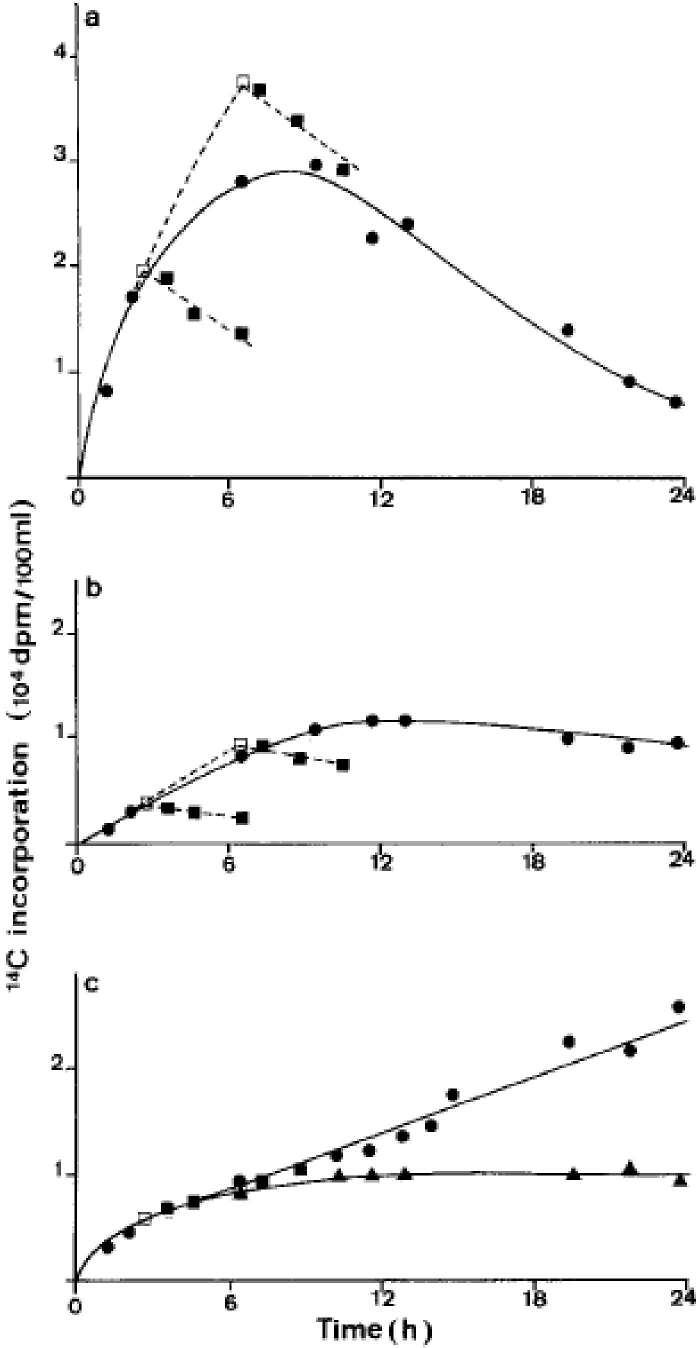


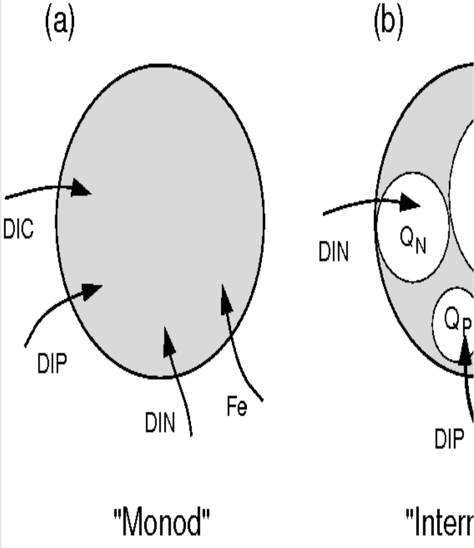
Fig. 6. Cumulative short-term light □ – dark ■ and long-term ● ^{14}C incorporation into (a) polysaccharides, (b) lipids, (c) proteins. Fig. 6c shows in addition long-term ^{14}C incorporation into small metabolites ▲

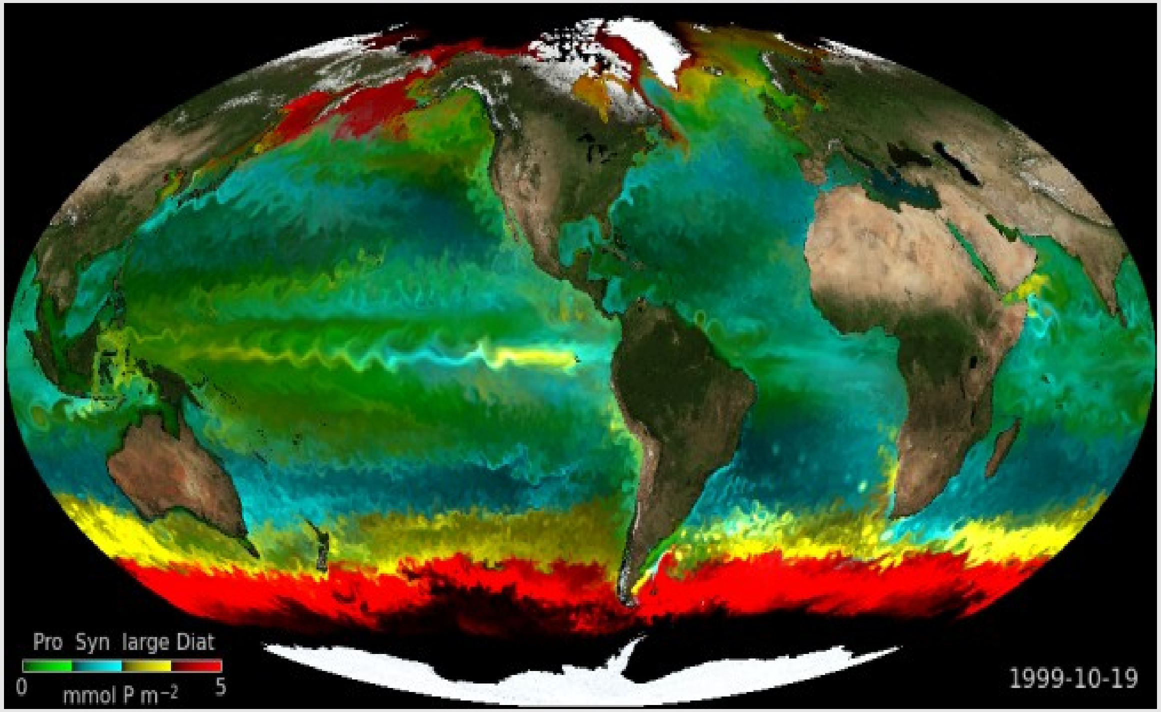
Lancelot and Mathot
Marine Biology 86, 219 (1985)

Numerous radiocarbon uptake studies can provide some appropriate constraints?

Computational limits allow 1000 state variables

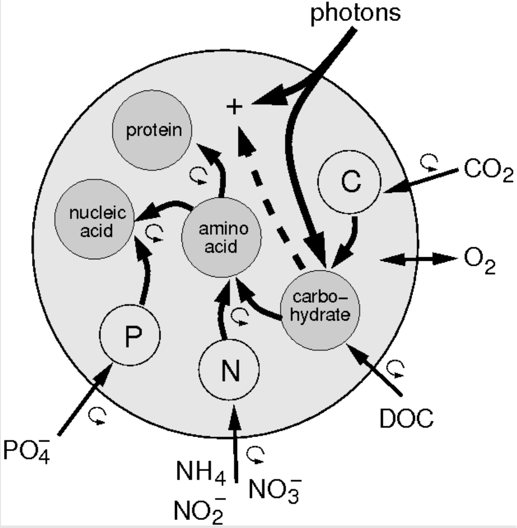
1000 cell types described by Monod kinetics

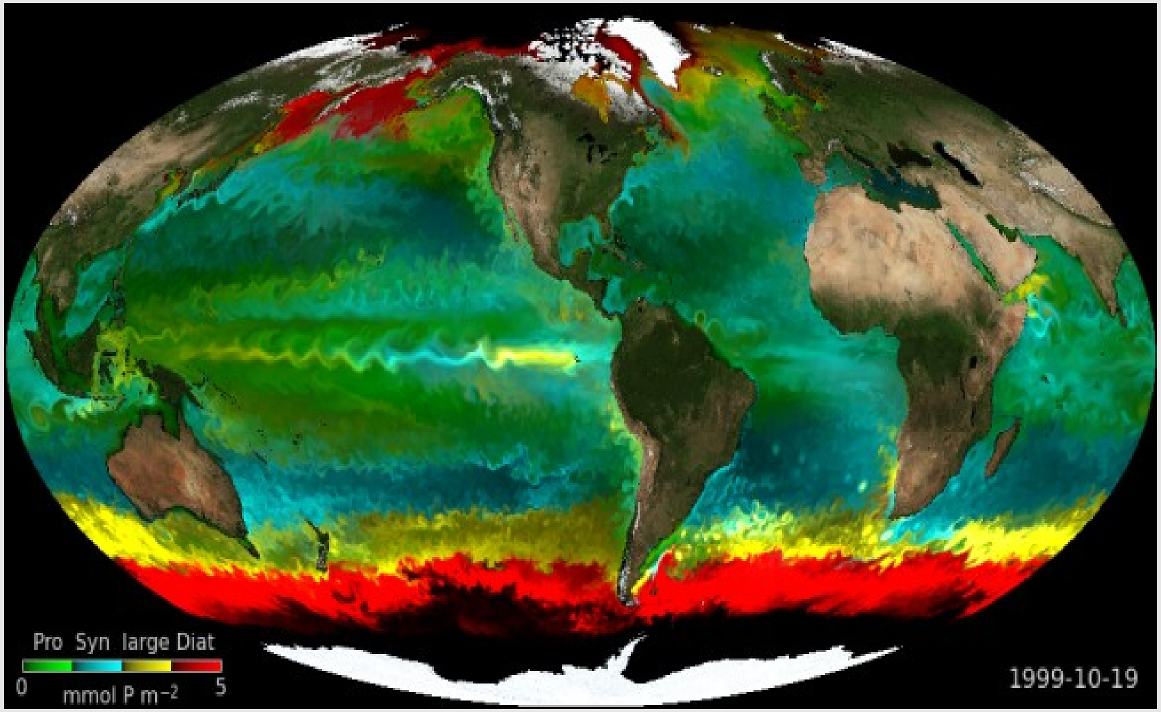




Computational limits allow 1000 state variables

~100 cell types described by "biochemical" model of cell

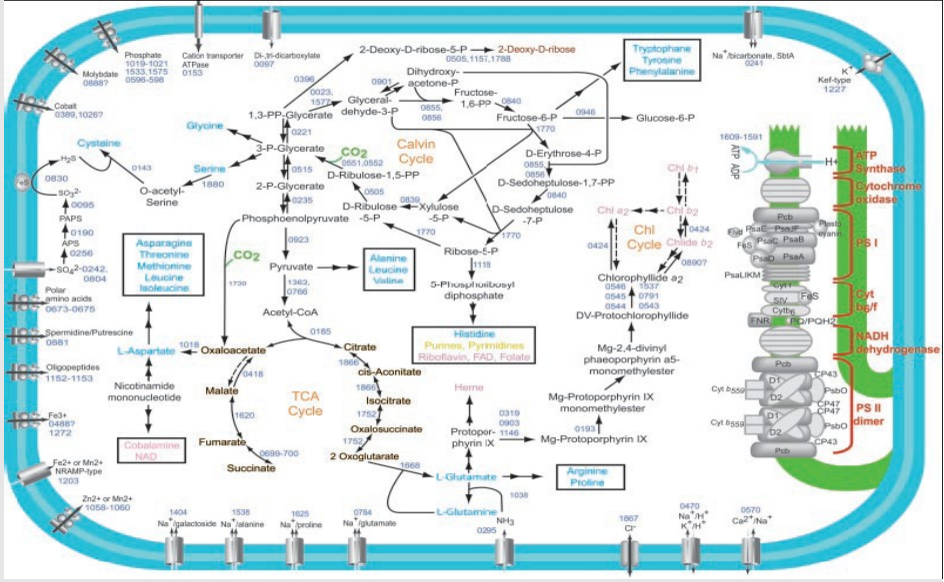


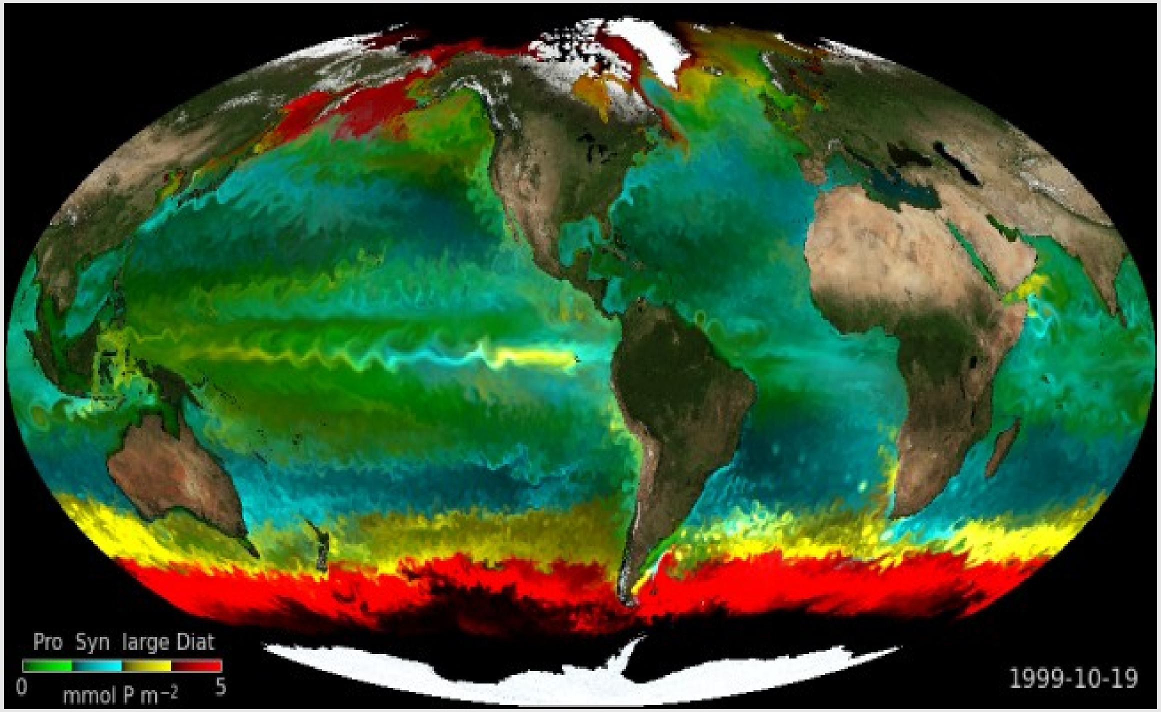


100 cell types
Each described by 10 (physiologically meaningful)

Computational limits allow 1000 state variables

~1 cell types described by 1000 state variables!





Summary

- Models provide a way to formalize and synthesize conceptual understanding
- Many models of marine microbial communities have their roots in studies of Fleming and Riley 80 yrs ago
- How will models relate to new “omics” perspectives of marine microbial communities?
  - continued Friday...