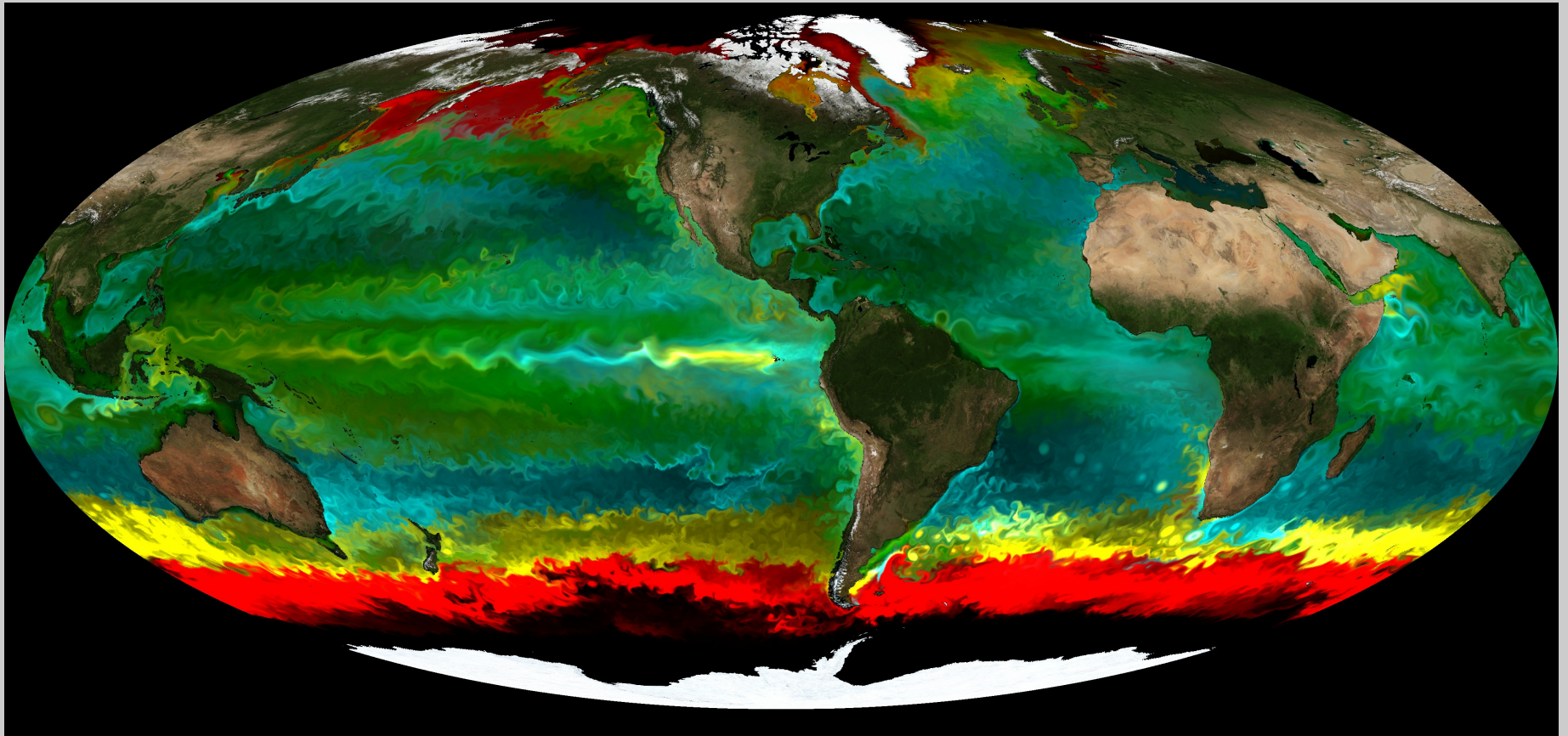
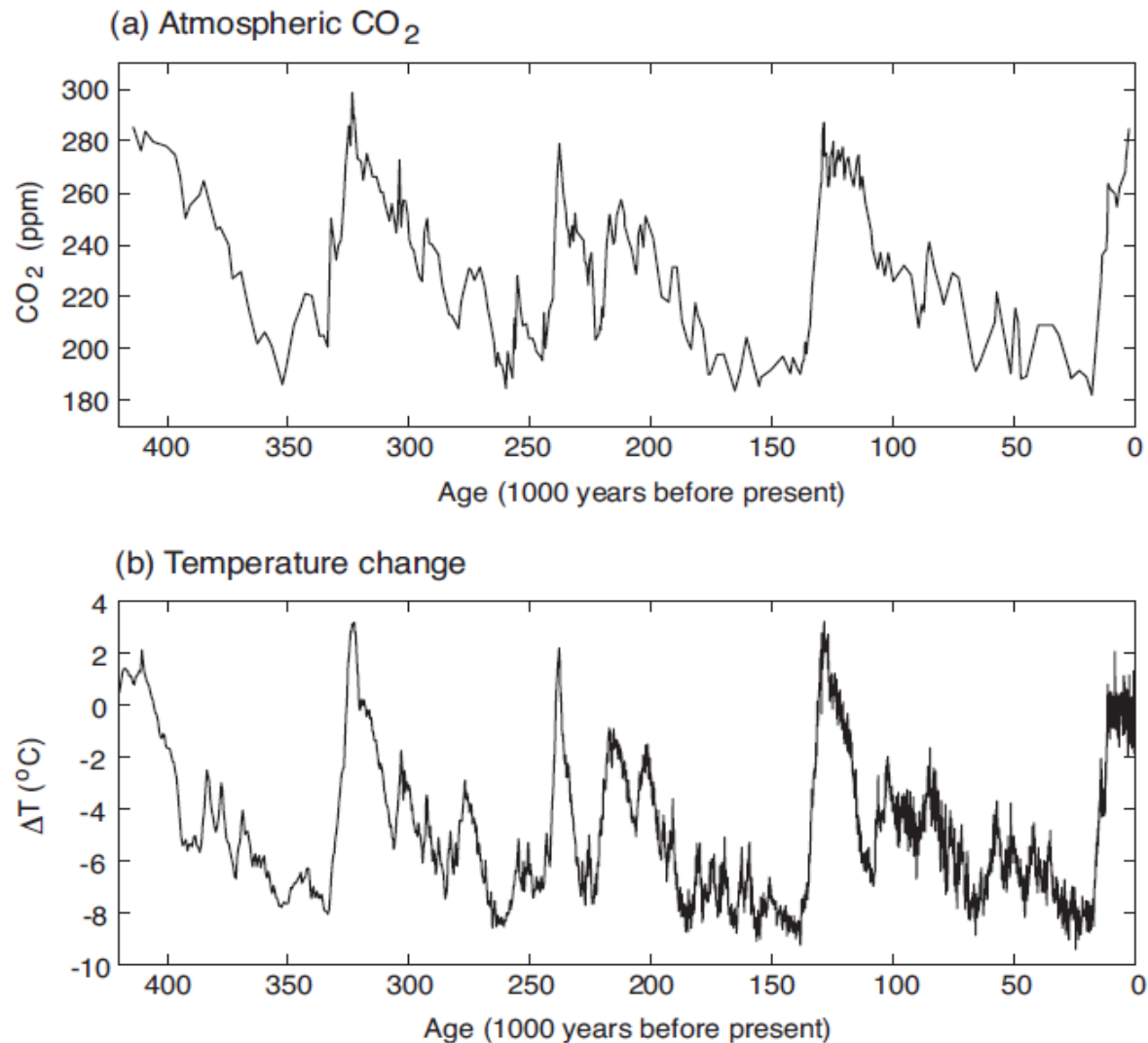


Global Modeling: Challenges and Opportunities



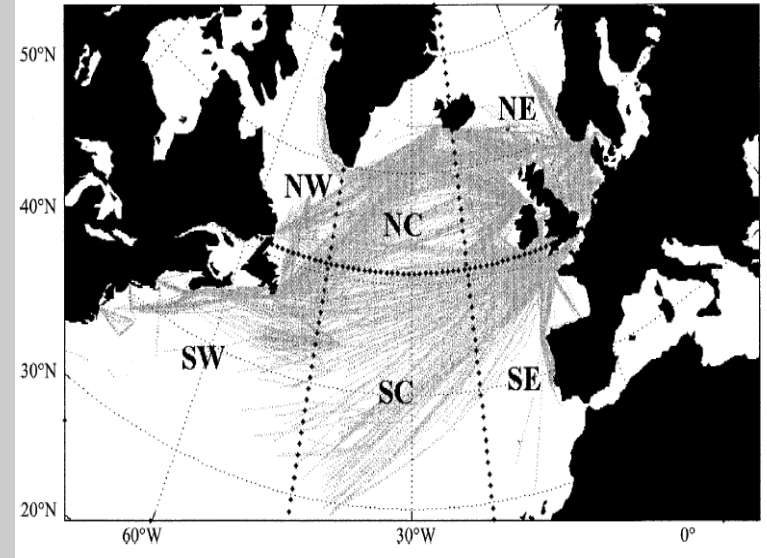
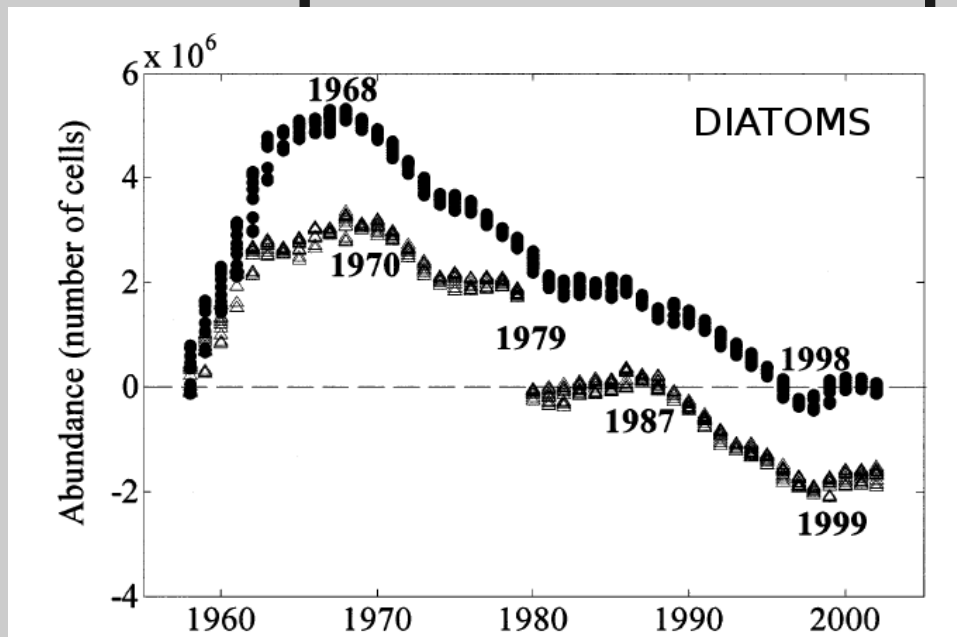
Mick Follows

Glacial-interglacial variations in atmospheric CO₂ and climate



Vostok ice core
(Antarctica)
Petit et al (1999)

Temporal variability of primary producers - phytoplankton



Sir Alistair Hardy

Continuous Plankton Recorder Survey
50+ years of opportunistic obs

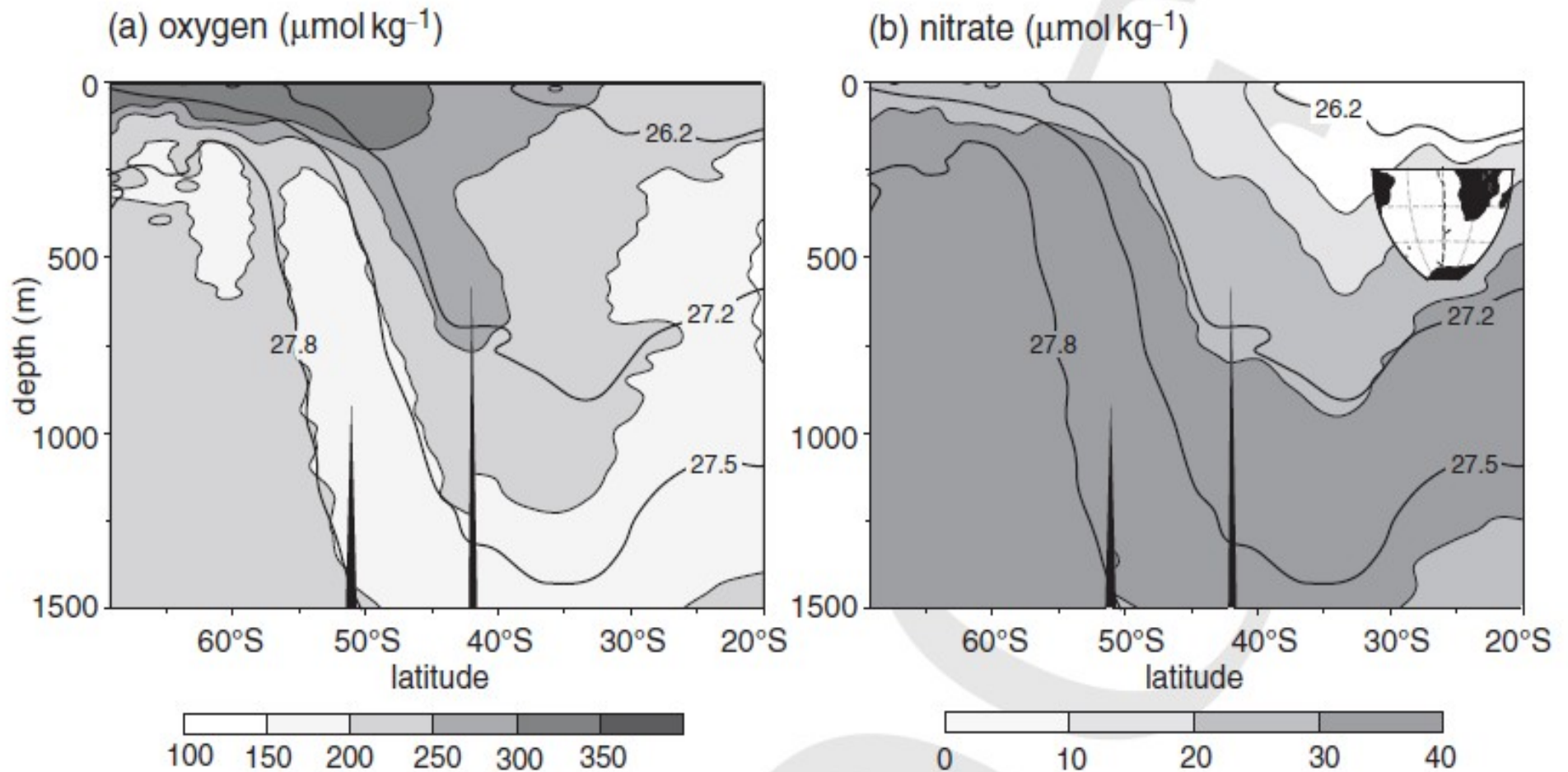
Leterme et al (2005)

- *What drives the changes?*
- *Environmental and ecological controls?*
- *Biogeochemical consequences?*

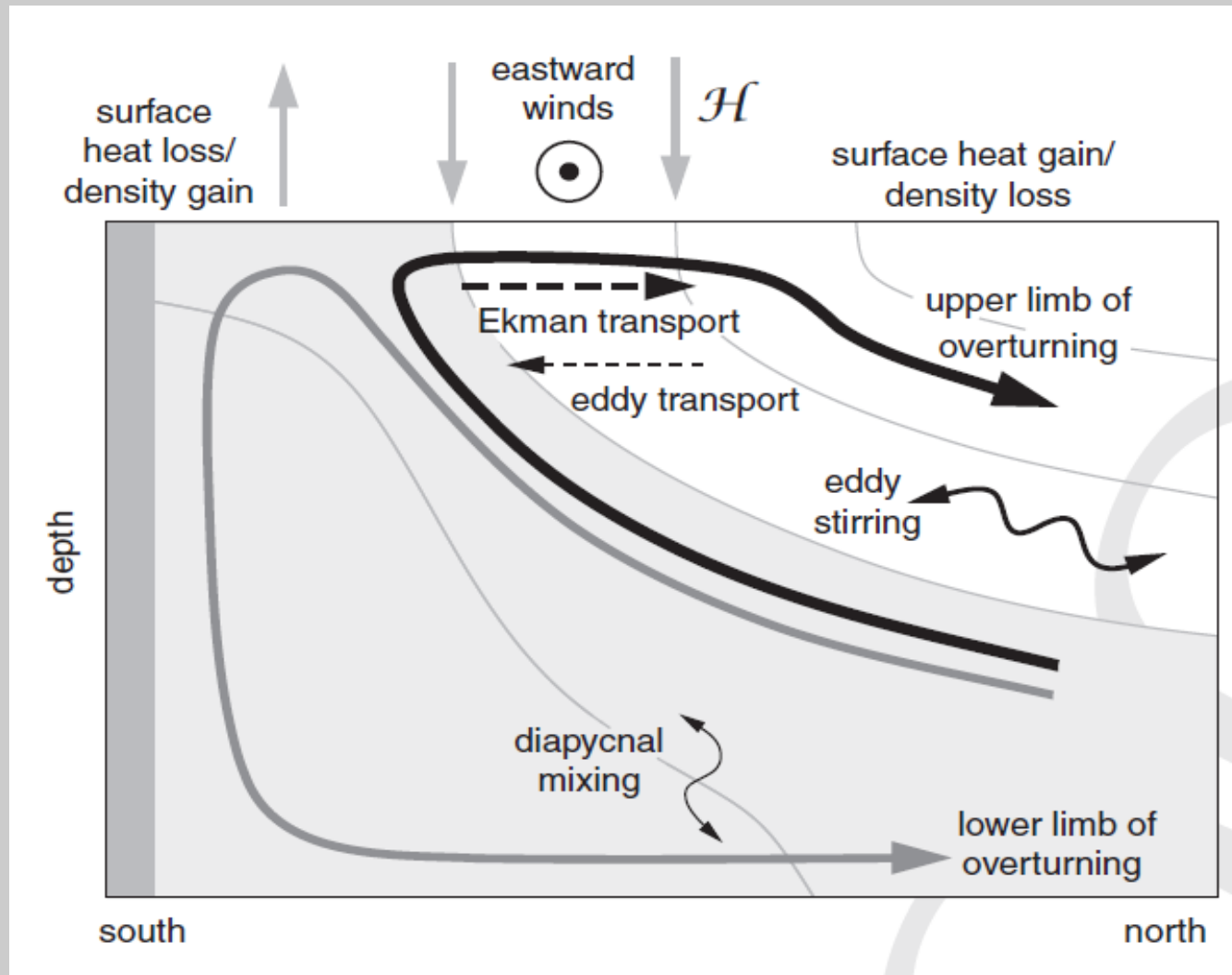
A significant global modeling challenge is to bridge the significant scales...

- Physical scales:
 - Molecular diffusion/viscosity to global overturning
- Biological scales:
 - Intra-cellular metabolic networks to global biogeography

Southern Ocean Circulation and Biogeochemistry



Southern Ocean Overturning and Tracer Transport

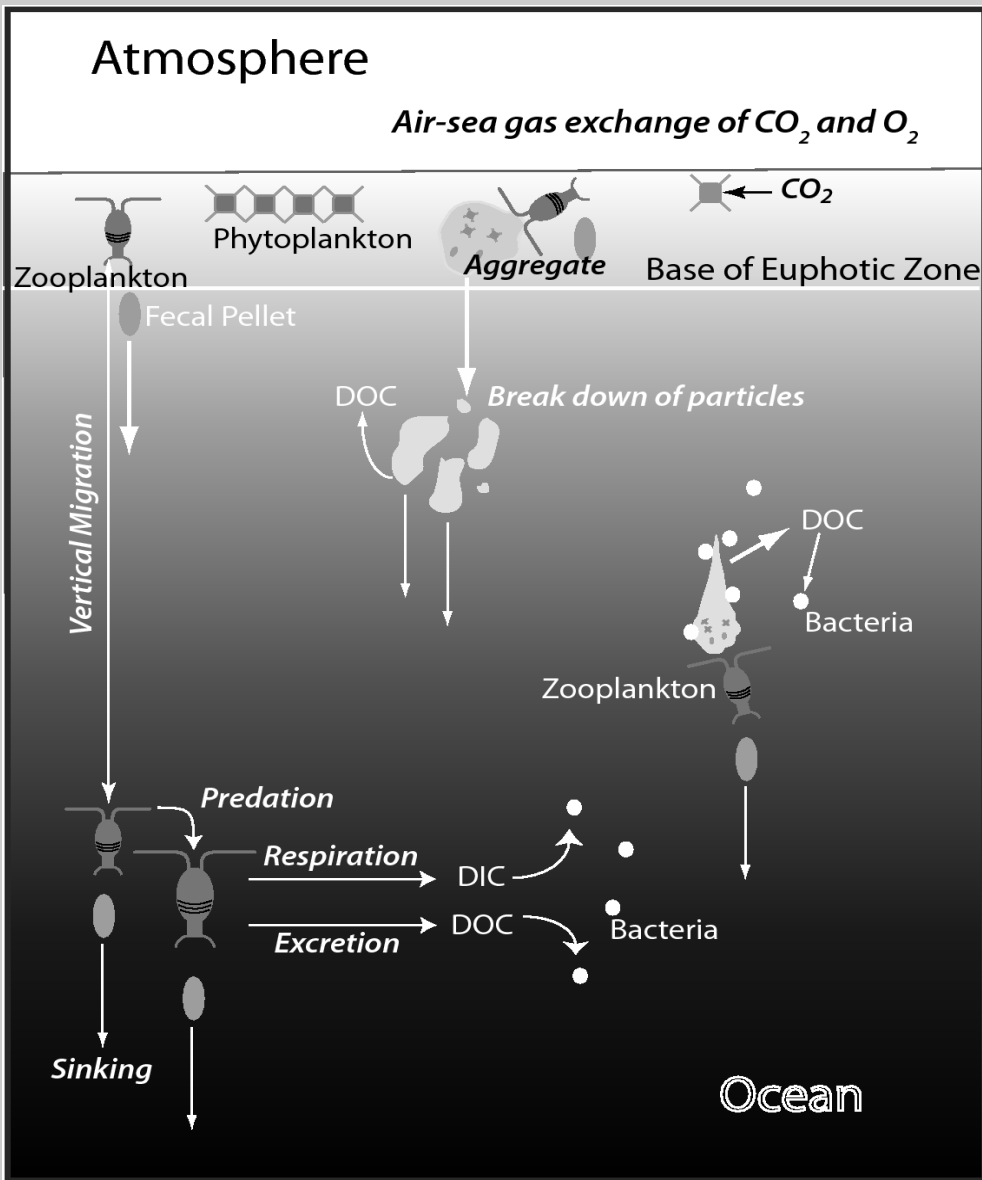


Challenge:

Modeling the range of physical scales significant for ocean circulation and climate variations

- Understanding, quantifying and parameterizing role of “fine scale” physical phenomena central to interpretation and simulation of global-scale circulation and its interaction with climate and biogeochemical cycles...

Food Web, Export and Carbon Cycle



Export of organic carbon and marine storage of carbon mediated by marine ecosystem

- Rate of primary production
- Character of primary producers
- Predation of primary producers
- Respiration of organic matter zooplankton
- Respiration by heterotrophic microbes
- Depth of respiration...

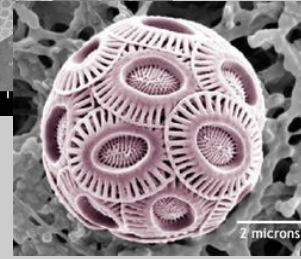
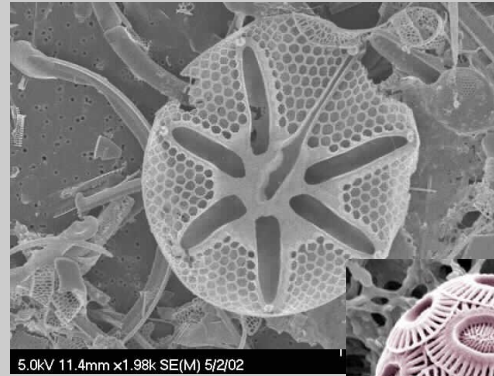
A challenge:
Understanding and modeling the
global biogeography of primary
producers and heterotrophic
microbes

How is it governed by the constraints at the scale
of individuals?

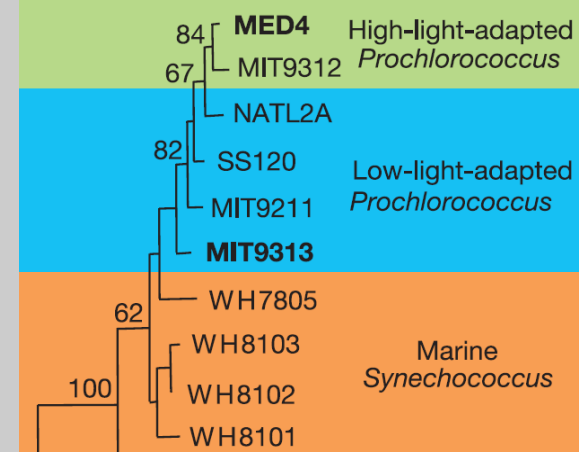
Biogeography of diverse primary producers

Significance:

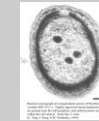
- Biogeochemical
 - export
 - DMS production
 - calcification
 - nitrogen fixation
- Ecological
 - Stability
 - Paradox of the plankton



- diatoms
- coccolithophorids

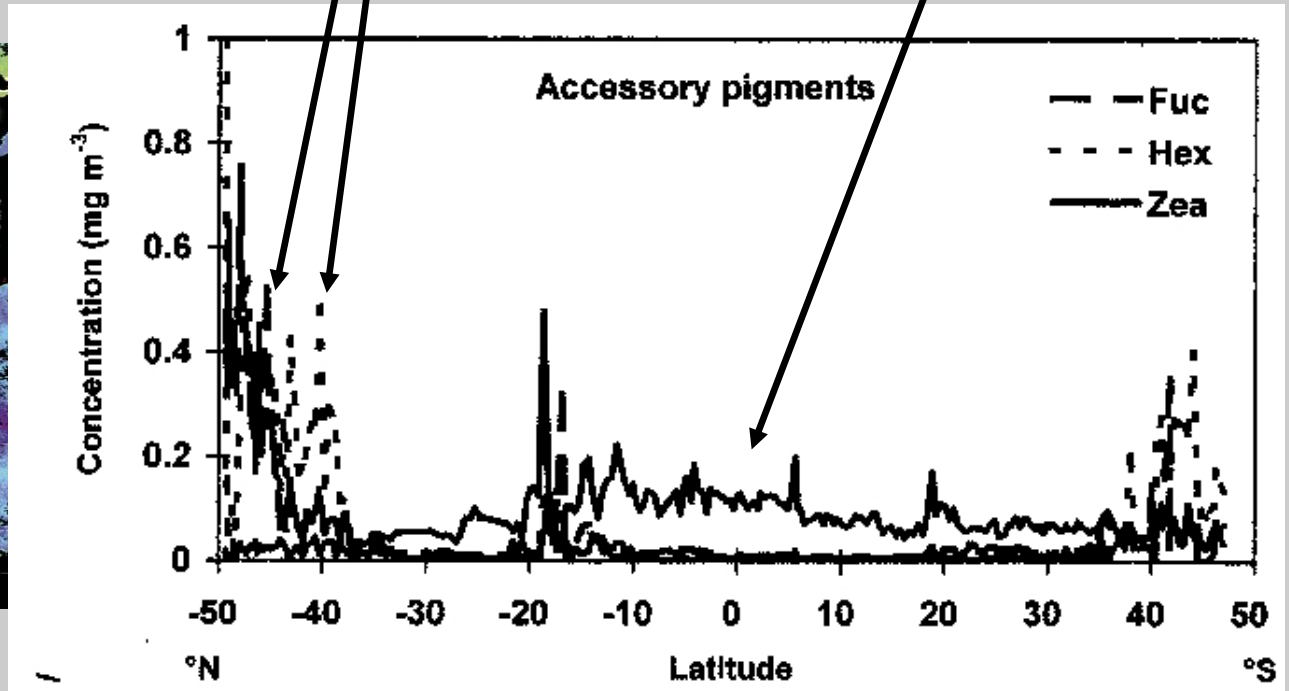
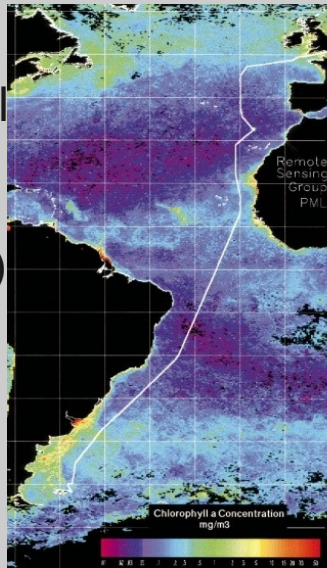


- pico-cyanobacteria
 - *Prochlorococcus*
 - *Synechococcus*

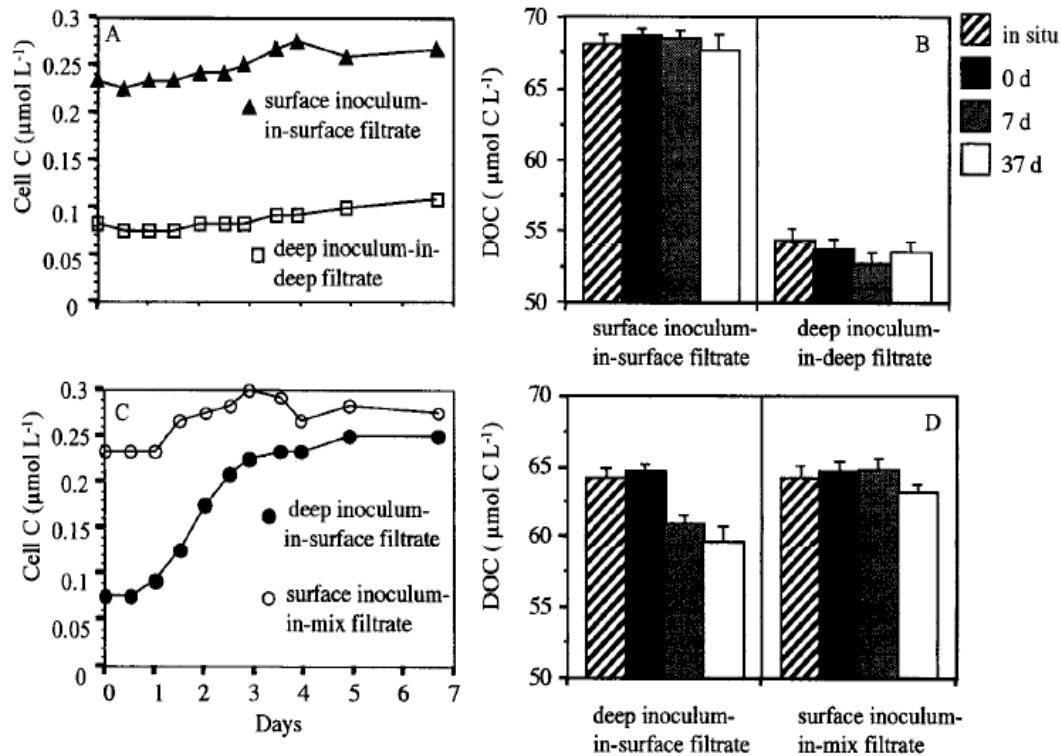


Atlantic Meridional
Transect (AMT):

Aiken et al. (2000)



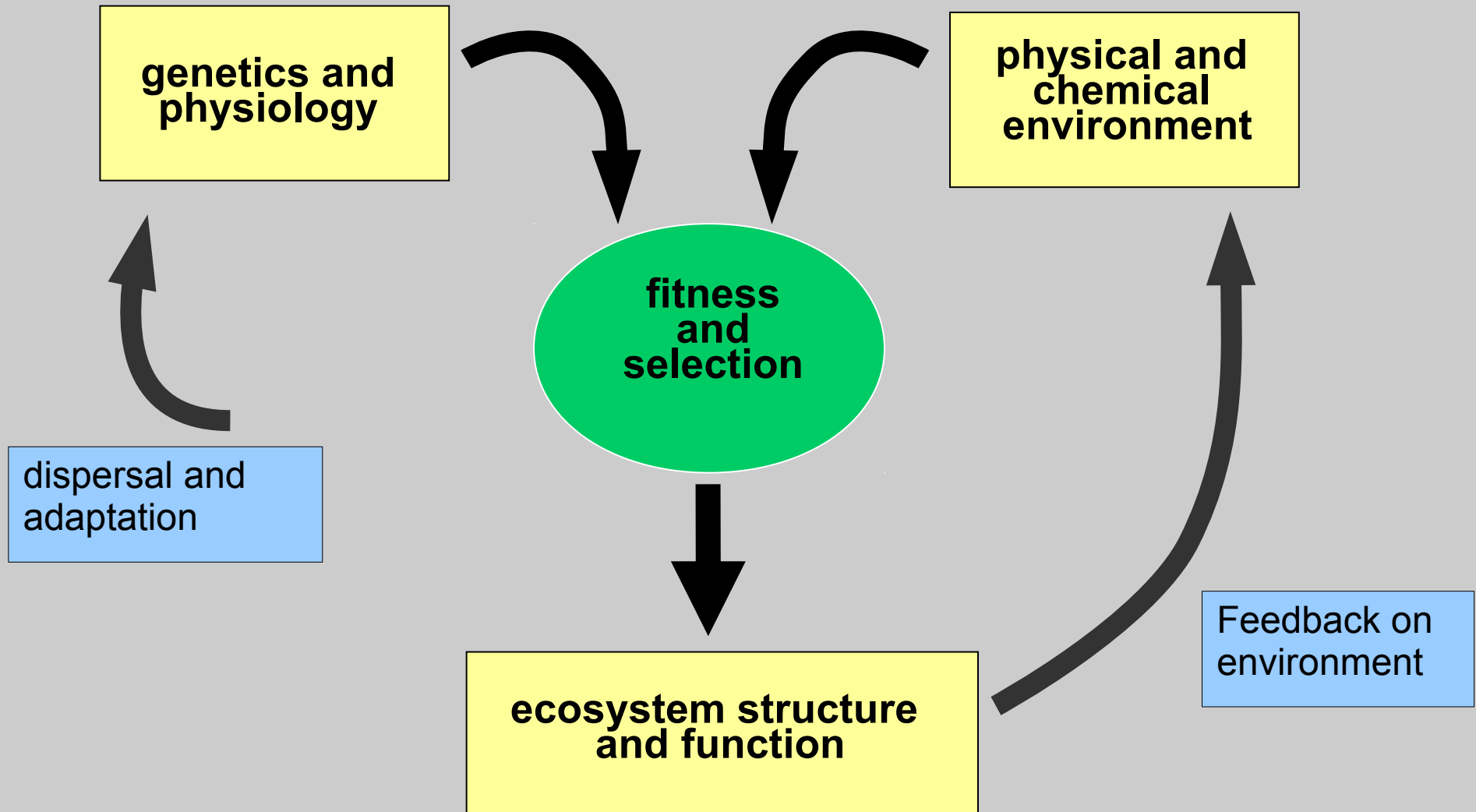
Biogeography of diverse heterotrophic microbes



- Diverse bacterial populations
- e.g. bacteria from surface and 250m have different substrate affinities
- “biogeography” of heterotrophic microbes related to resource distributions
- Implications for rates of respiration of “labile” and “semi-labile” DOC

Carlson et al (2004)

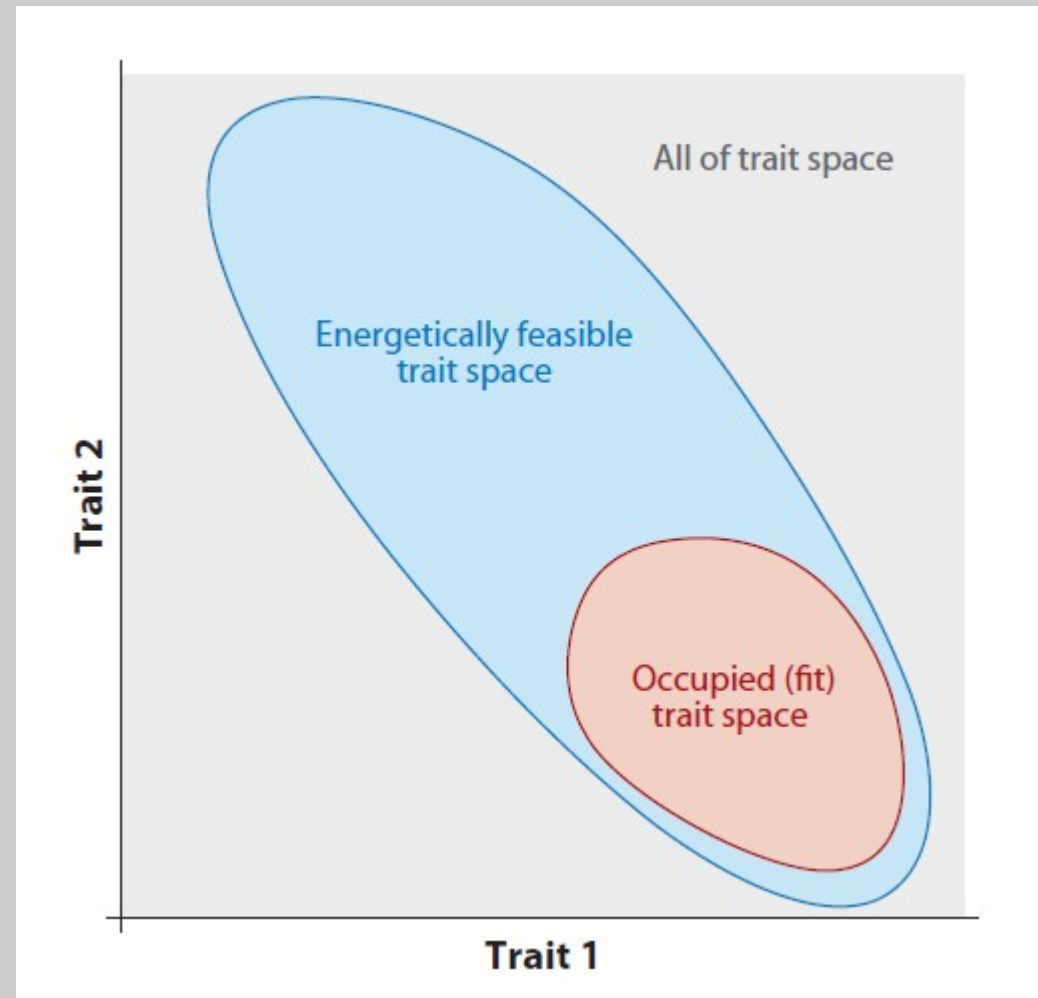
A guiding principle for “trait-based” models of microbial communities



“Everything is everywhere but the environment selects” – Baas Becking (1934)

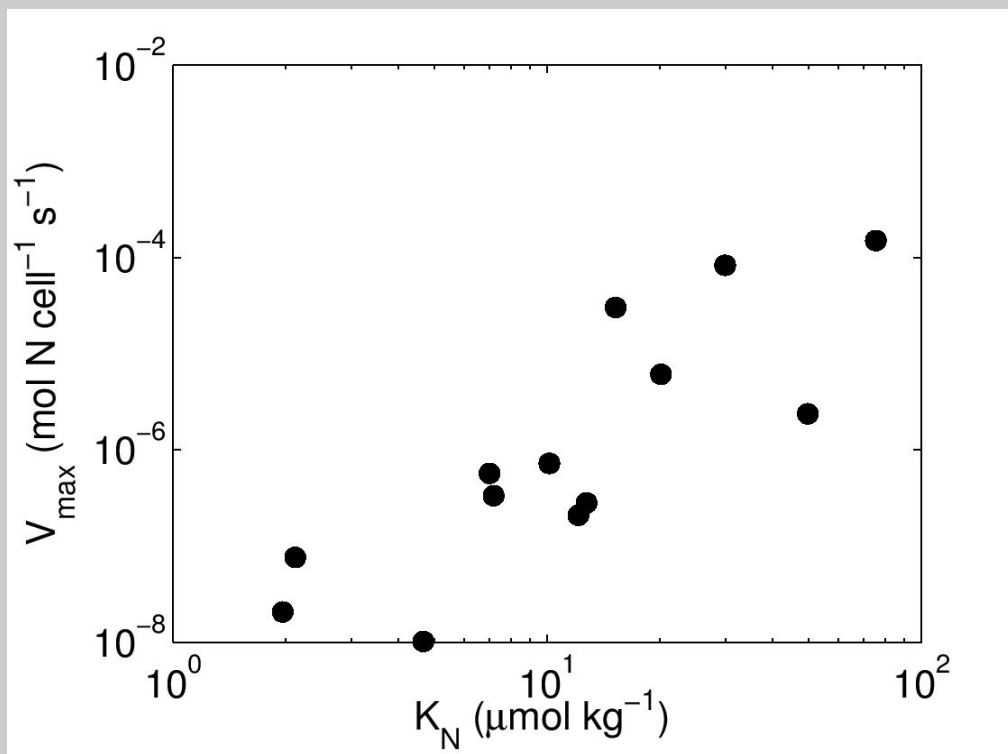
Modeling diverse ecosystems: Traits and trade-offs are critical

- What controls traits and trade-offs?
 - Organism size
 - Resource allocation at individual scale



Example: Trade-offs for nitrate acquisition

Litchman et al (2007)

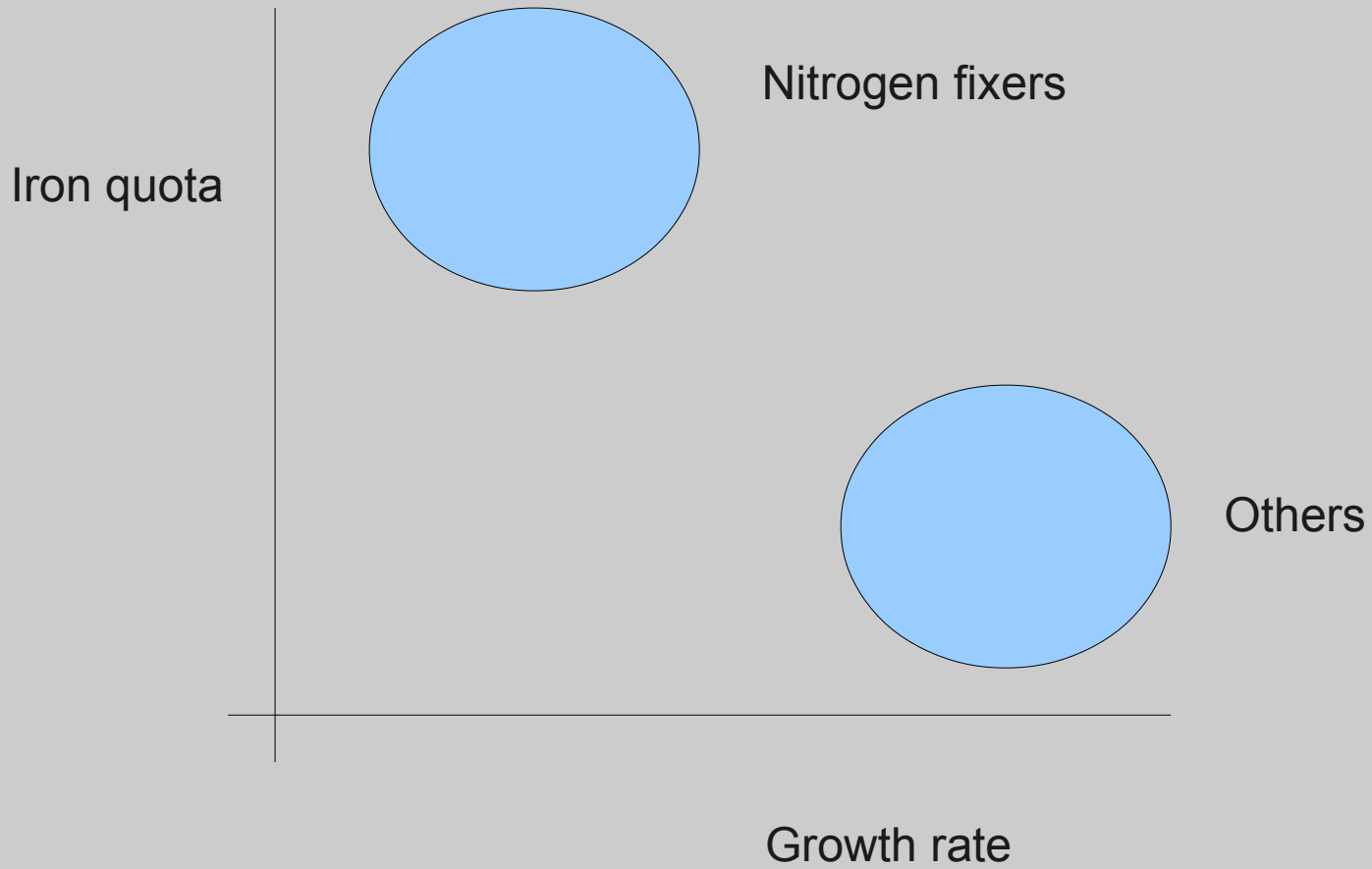


Example:

- Trade-off between maximum nitrogen uptake rate, V_{\max} , and half-saturation, K_N
- This trade-off mediated by cell size

Example: Nitrogen fixers

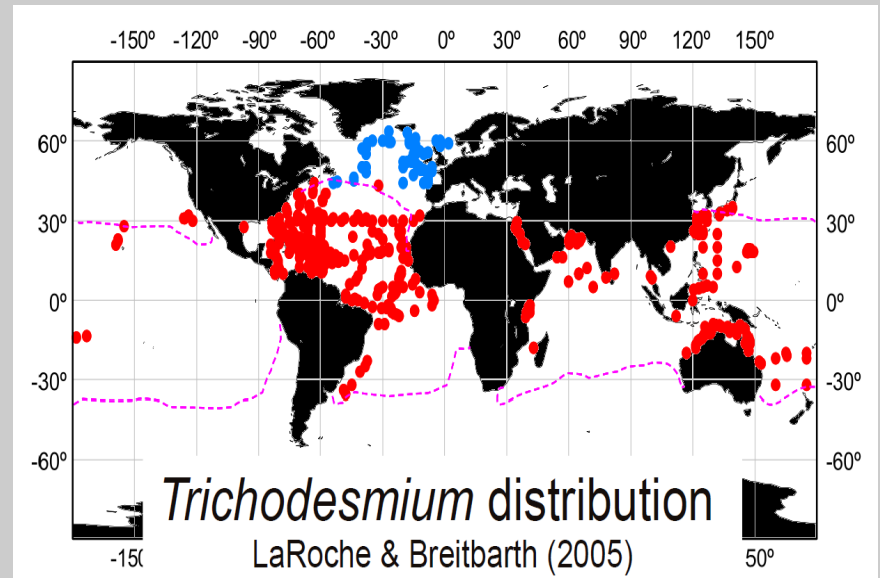
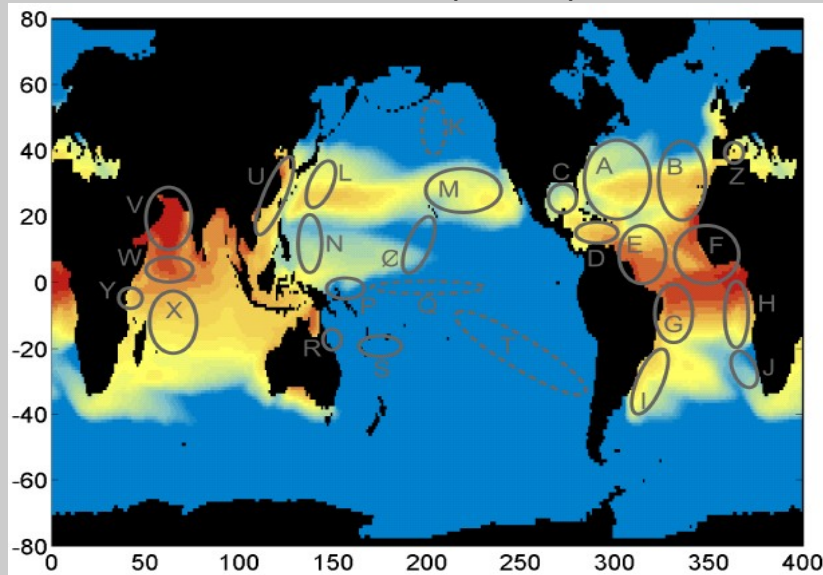
- Diazotrophs (nitrogen fixers) require additional iron for nitrogenase
- Diazotrophs have slower growth rate than non-nitrogen fixing counterparts
 - energetic cost of nitrogen fixation?
- *Resource availability and allocation determines ranges of diazotroph species (e.g. Saito et al., 2011)*



Example: Modeled biogeography of phototrophic diazotrophs

- Assumed trade-offs for diazotrophy
 - High iron quota
 - Low maximum growth rate
- Plausible biogeography emerges in competition with non-diazotrophs

e.g. Modeled diazotroph biomass
Monteiro et al (2010)



A challenge:

What are the traits and trade-offs which define fitness associated with calcification?

- Calcification of central importance in regulating global ocean biogeochemistry on vast range of timescales
- What are costs and benefits of calcification to the individual organism?
- How does environment (and its variability) regulate fitness of calcifiers?



A challenge:

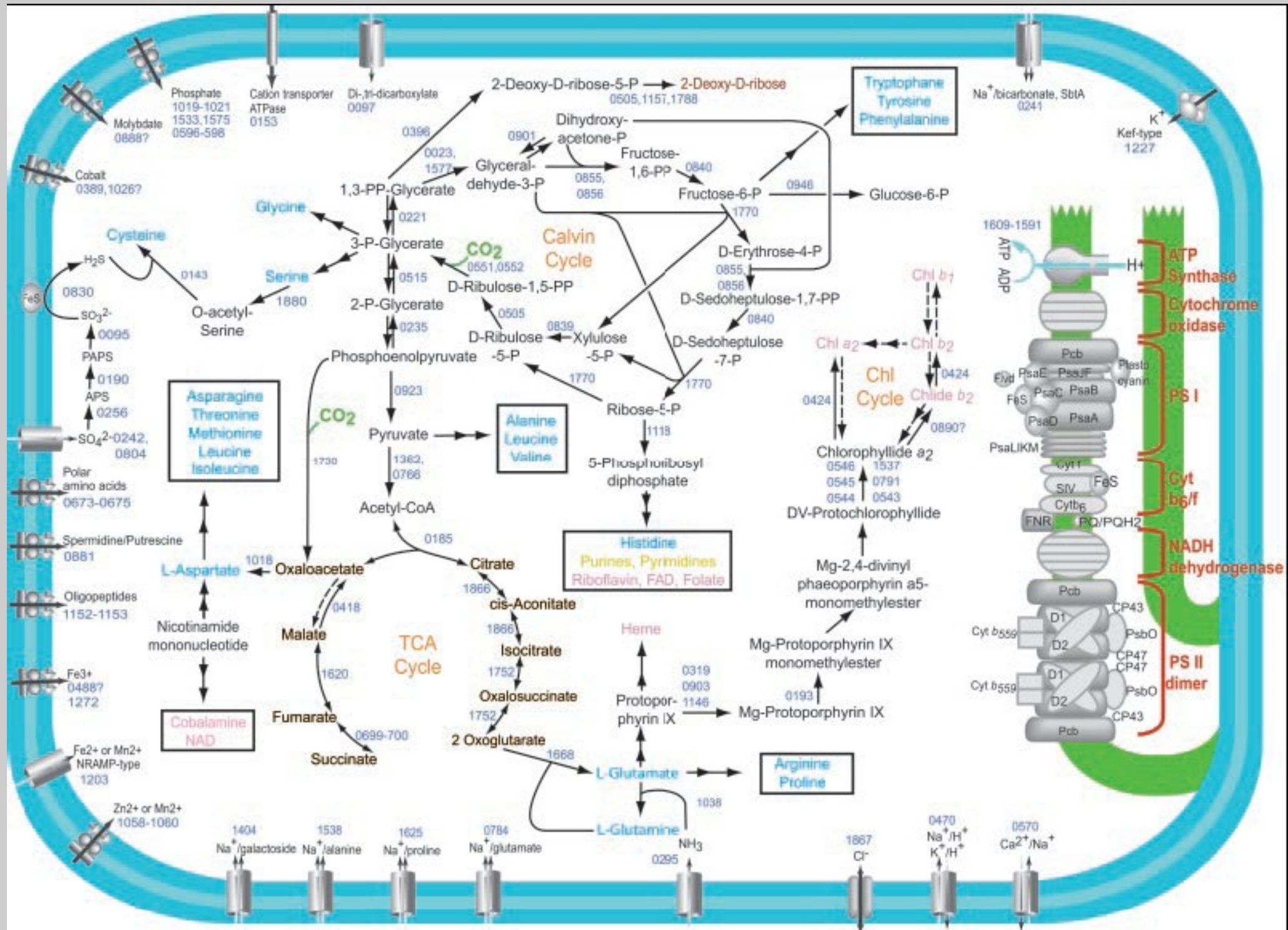
What are the traits and trade-offs which define the fitness and function of diverse heterotrophic microbes?

- Adaptation for specific substrates (i.e. Components of DOC and POC)?
- Size, morphology? (important for photo-autotrophs)
- *Implications for efficiency of recycling, export and storage of carbon*

The promise and challenge of molecular information

- Molecular biology has provided tools to identify and map traits, and association with organisms, in environment
 - e.g. micron-scale, unicellular diazotrophs
- Genomic characterization of organisms provides extremely detailed mapping of metabolic networks, flow of elements within cells
 - Information about resource allocation and trade-offs at the scale of individual

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



Whole cell metabolic models: e.g. Edwards et al (2001)

In silico predictions of *Escherichia coli* metabolic capabilities are consistent with experimental data

Jeremy S. Edwards^{1,2}, Rafael U. Ibarra¹, and Bernhard O. Palsson^{1*}

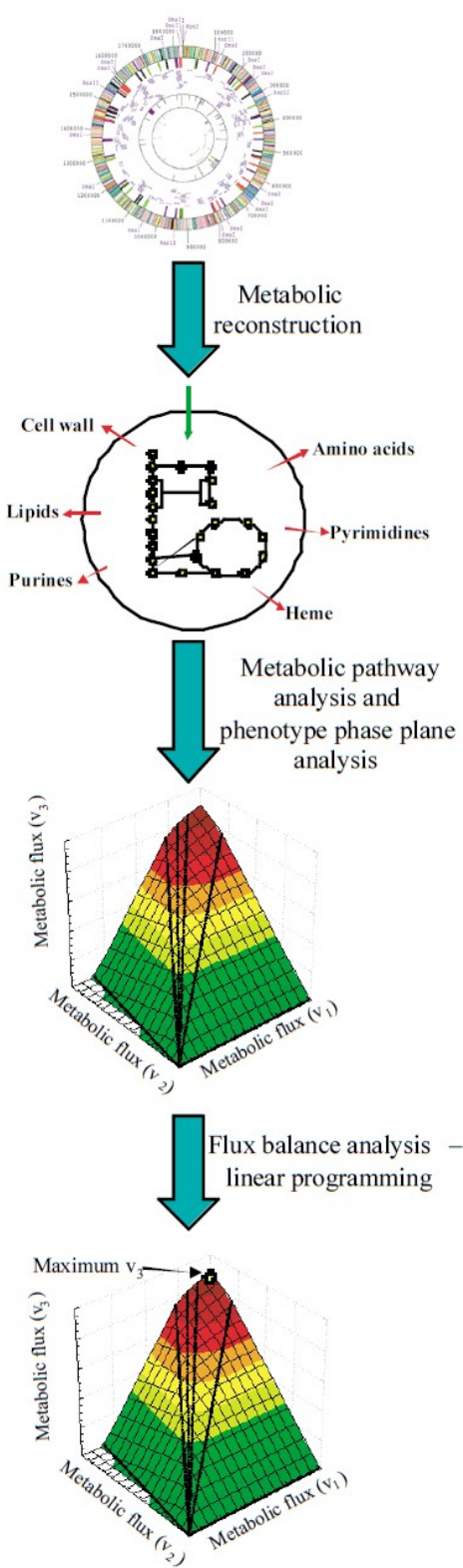
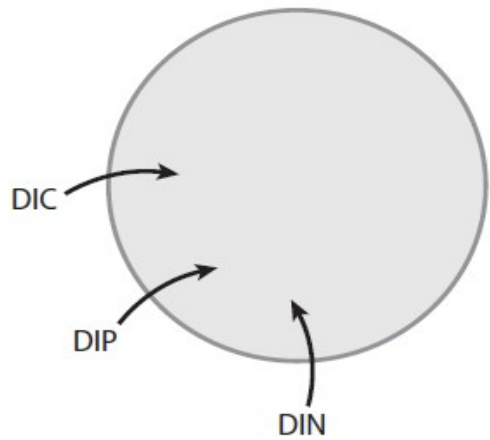


Figure 1. From genome sequence to metabolic characteristics. The metabolic network can be reconstructed from the annotated genome sequence^{2,5,51}. The global properties of the metabolic reconstruction can be studied to determine the feasible steady-state metabolic flux distributions, and this process can be performed with a whole-cell pathway analysis^{34,35}. However, this process is computationally intense; thus we can map feasible steady-state metabolic flux distributions using an alternative approach known as phenotype phase plane (PhPP) analysis^{7,31,36}. PhPP analysis consists of calculating the optimal solution using linear programming as a function of two fluxes in the metabolic network (by setting the α and β value in equation 1). This process constructs the surface revealed in the figure. Finally, linear programming can be applied to calculate the value of the objective function for specific values of the uptake fluxes; additionally, the optimal value of all other fluxes is calculated^{26,29,30}. The results from this process can be compared to experimental data to evaluate the suitability of this modeling framework. Furthermore, this modeling approach can be used to guide the metabolic engineering of industrial microorganisms.

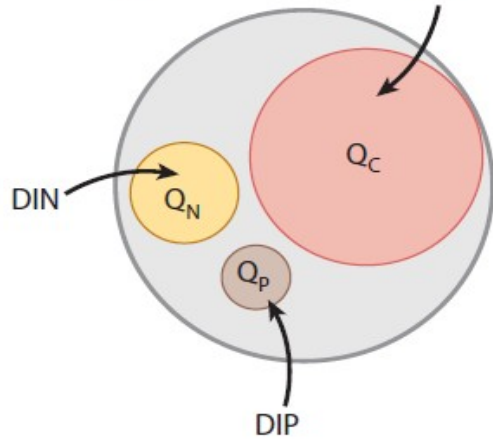
Cross-scale modeling of marine microbial populations and biogeochemical cycles

- Processes at individual level may be mapped and constrained by conservation of mass and energy
- Defines, in part, fitness in a given environment
- *Must be simplified and parameterized for practical application in large scale ecological and biogeochemical models.*
- ***Analogy to modeling physical circulation of ocean***

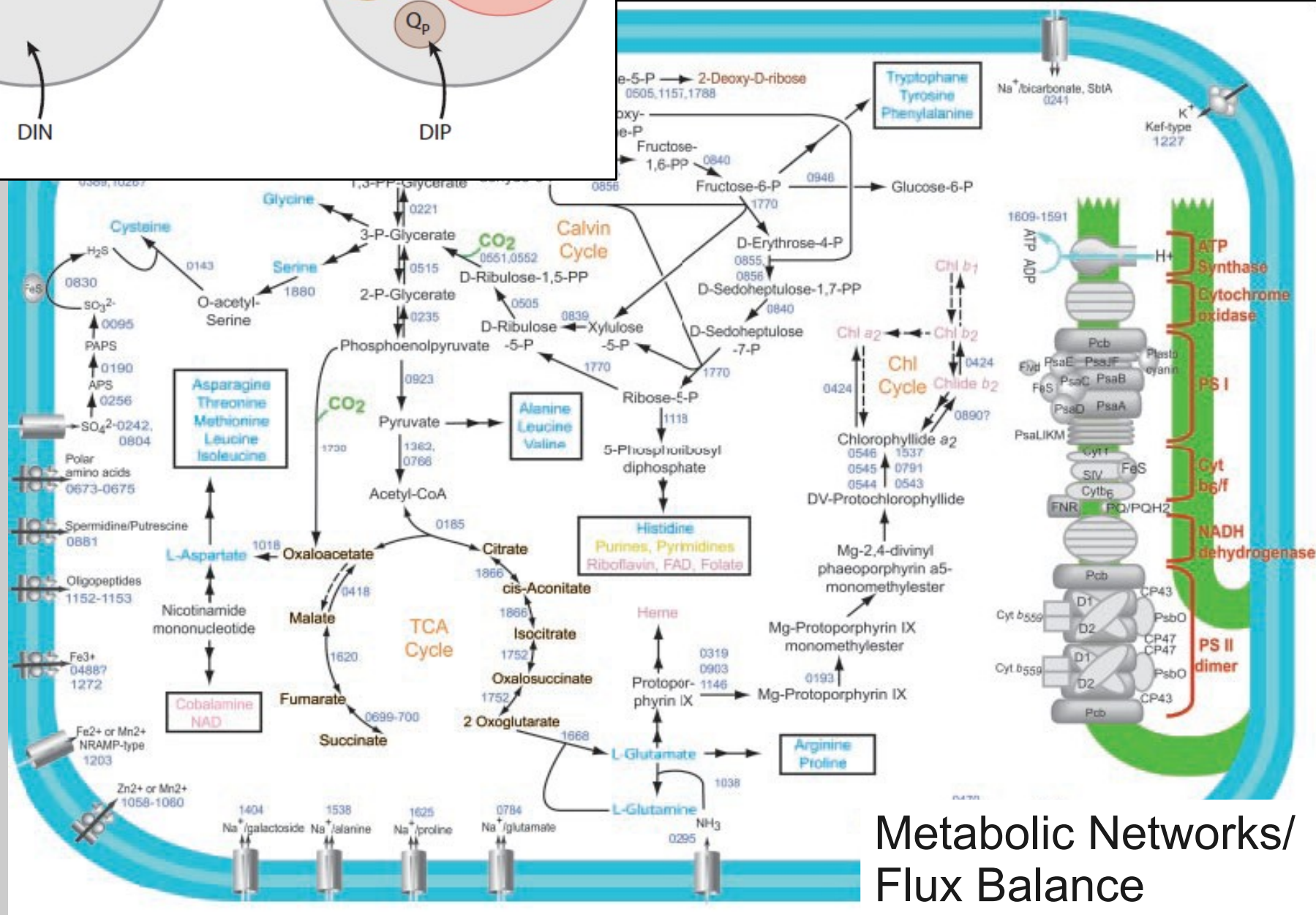
Monod/Redfield



Internal stores

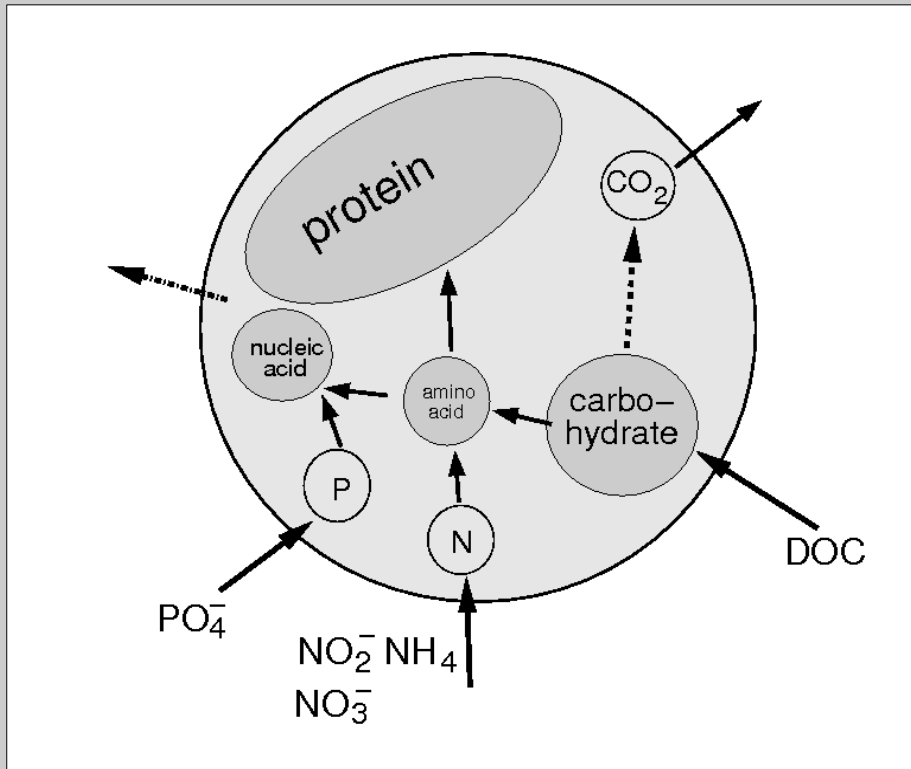


Physiological models



Metabolic Networks/
Flux Balance

An intermediate approach: Resolving macromolecular composition, elemental and energy flow



- *Explicit energy and mass constraints*
- *Macromolecular elemental composition prescribed*
- *Whole cell elemental composition dynamic*
- *models of similar nature published in bio-engineering literature*

Examples: Shuter (1979), Shuler et al (1979), ...

Summary

- Characterizing and quantifying “traits and trade-offs” at the scale of individuals is a critical step in advancing “trait-based” representations of marine ecosystems and biogeochemical cycles
- Detailed conservation constraints at the cellular scale can provide the basis for key trade-offs
- Genomic and molecular approaches provide information at the cellular scale
- ... but parameterization is necessary (essential?) for global, climate scale studies
- There is parallel with the tension between understanding, resolving and parameterizing fine-scale physical phenomena in climate models

Food webs and fisheries

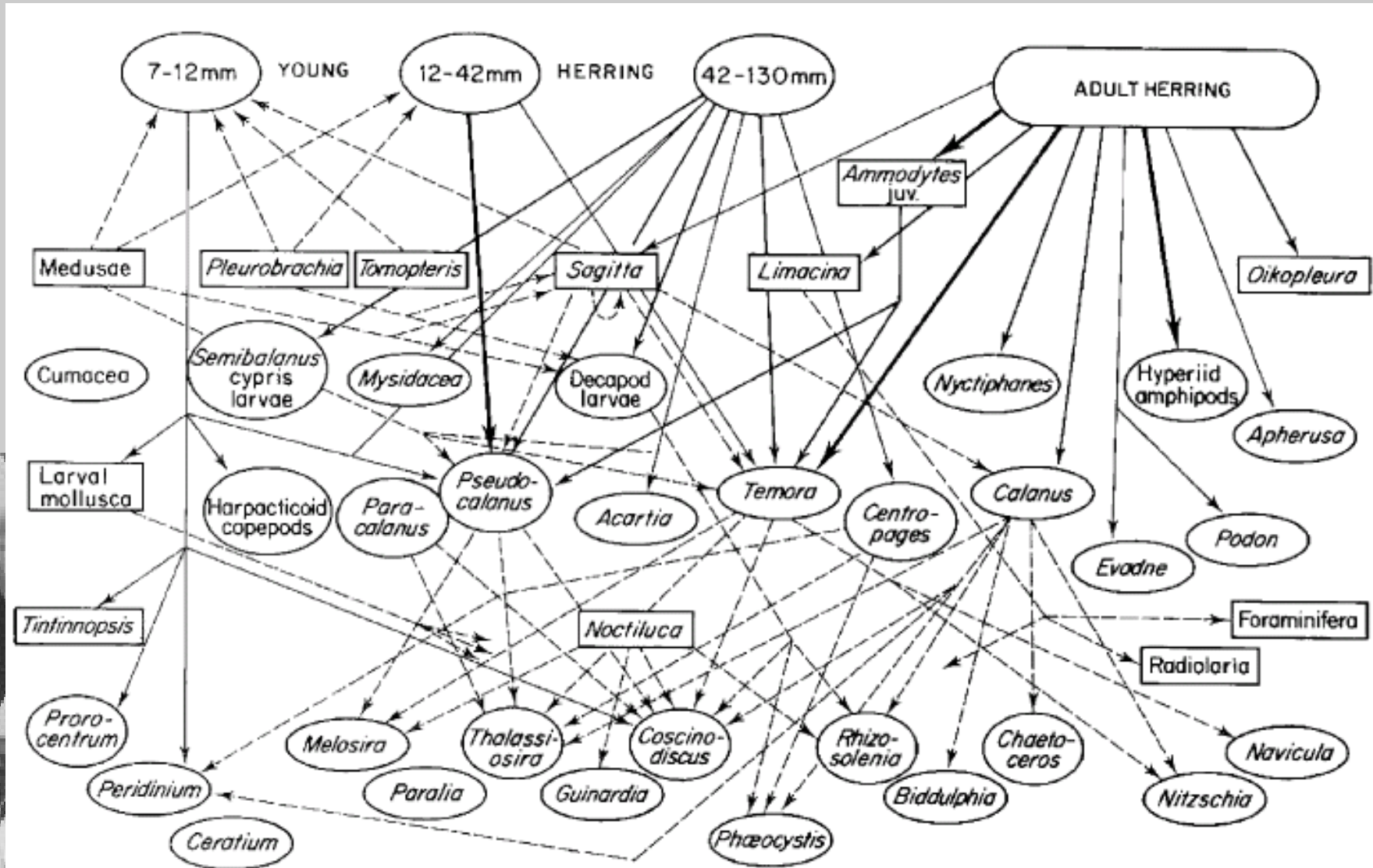
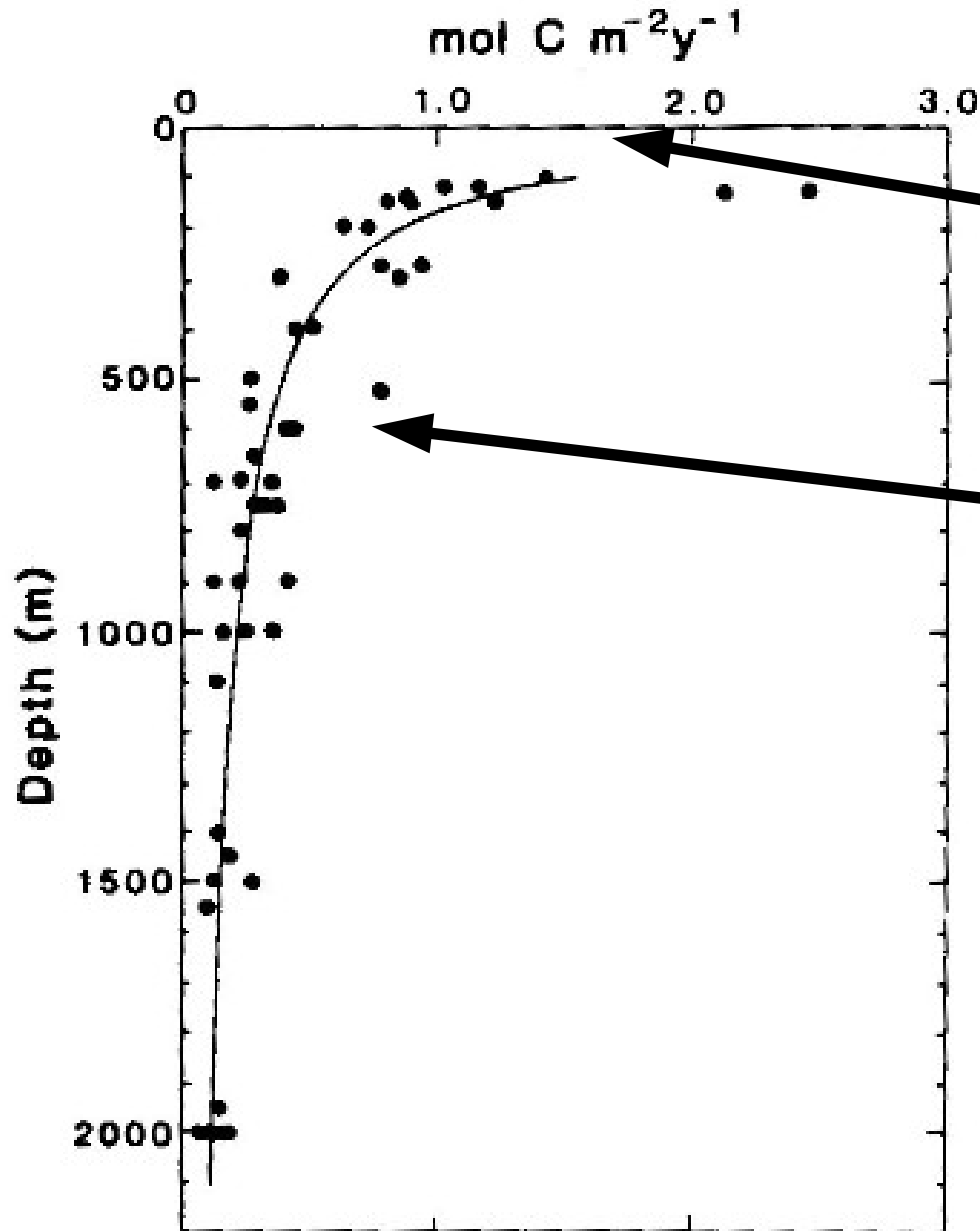


Fig. 4. The food web of herring *Clupea harengus*. From Hardy (1924).

Sir Alister Hardy (1924)

Redrawn by Brander et al (2003)

Biologically driven downwards transfer of nutrient elements (C, N, P, Fe, ...)

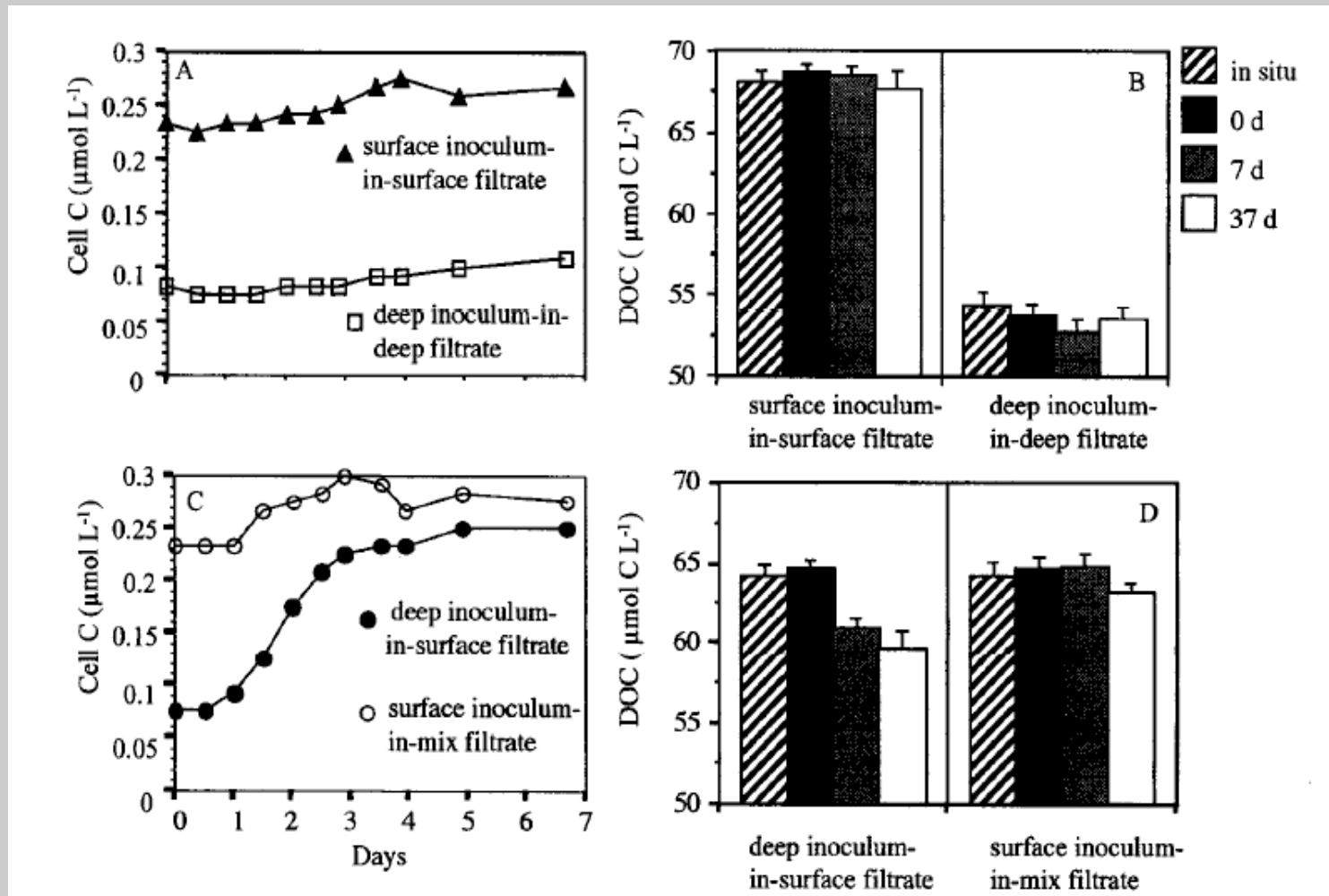


Photosynthesis & production of sinking organic particles

Respiration and re-mineralization by zooplankton & heterotrophic microbes

- Martin et al. (1987)
- Sinking flux of particulate organic carbon through water column

Respiration and the character of organic matter



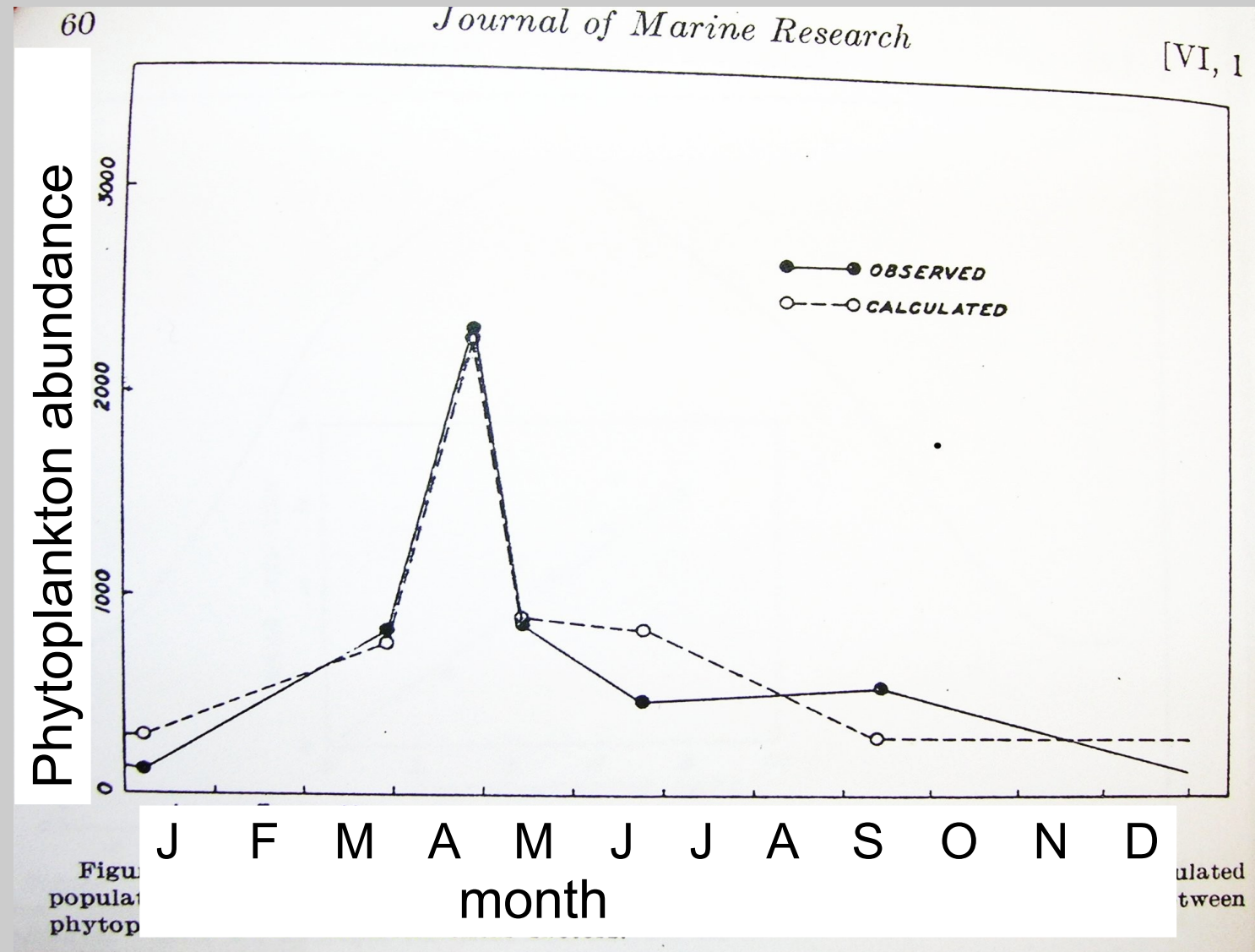
Carlson et al (2004)

An interesting historical parallel

- Gordon Riley (1946) sought to understand complex relationships between phytoplankton abundance and environment at Georges Bank introducing mechanistic models to complement statistical models.
 - Analogous situation with metagenomic data – currently not well connected to mechanistic models.

Modeling seasonal variations in marine phytoplankton: Riley (1946) JMR 6

Statistical model



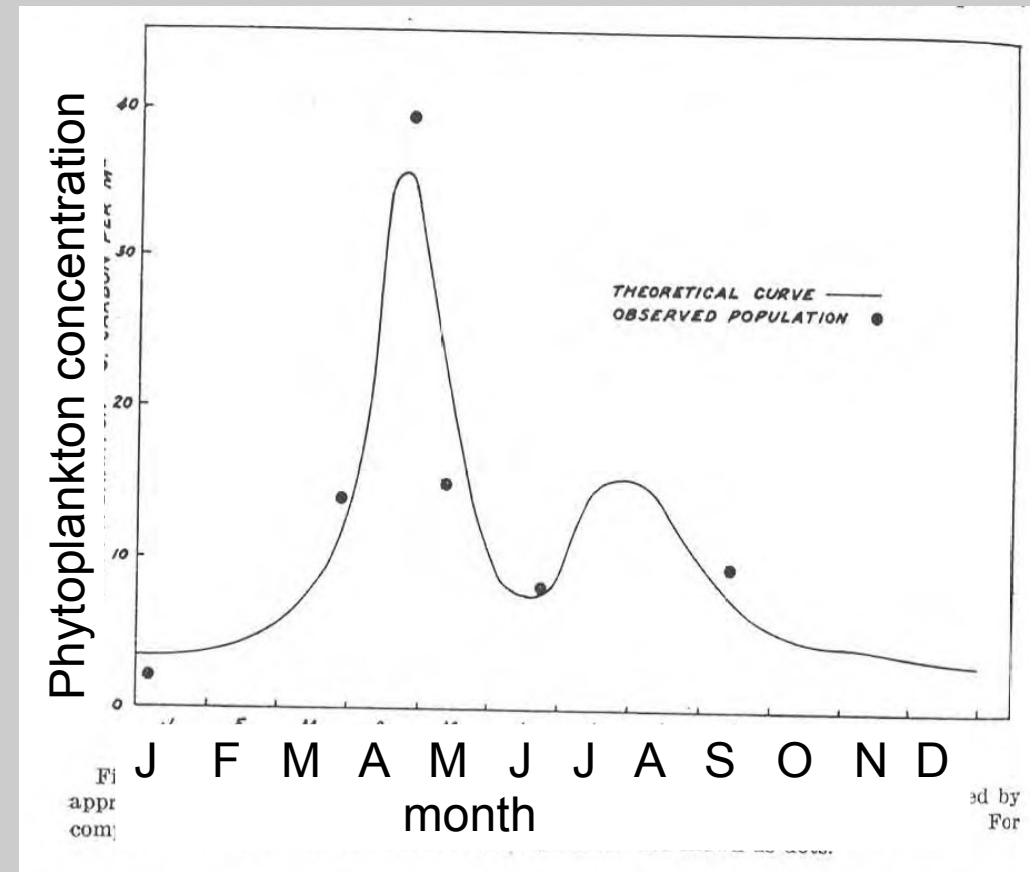
Modeling seasonal variations in marine phytoplankton: Riley (1946) JMR 6

$$\frac{dP}{dt} = \mu P - K P - g Z P$$

growth respiration grazing

rate of
change

**Dynamic
model**



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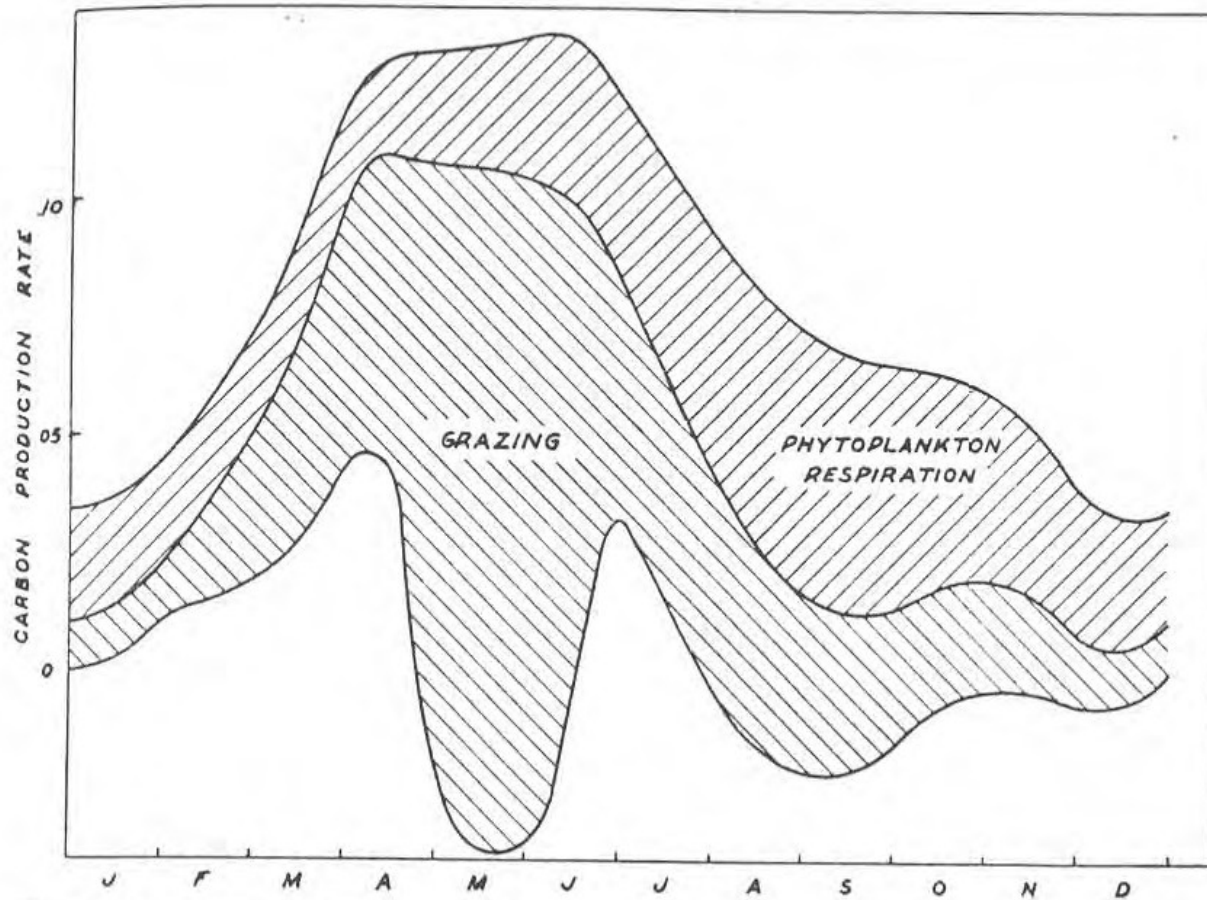
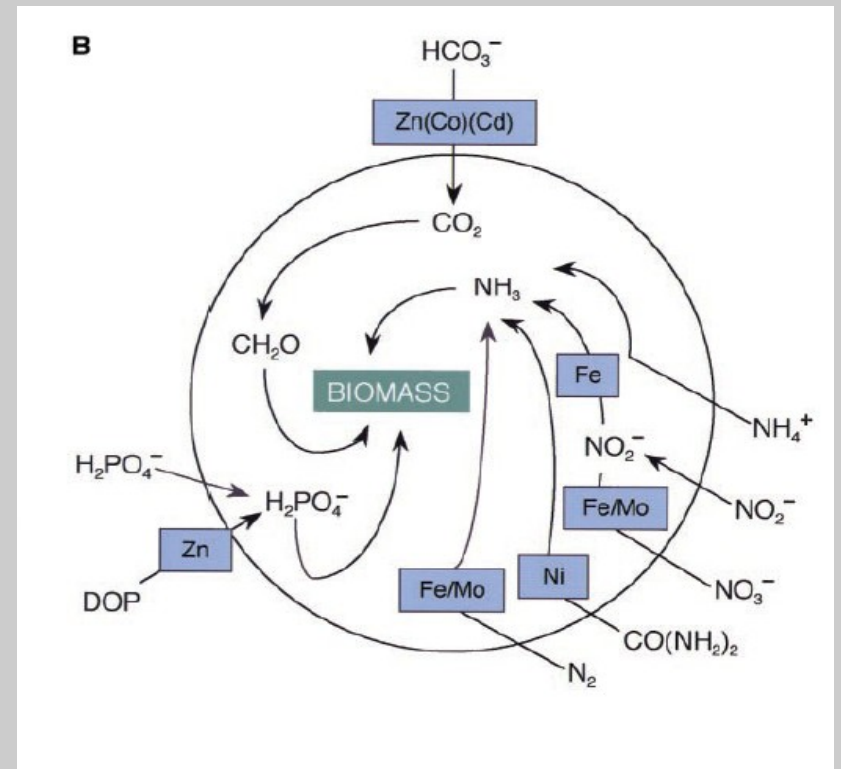


Figure 20. Estimated rates of production and consumption of carbon. Curve at top is the photosynthetic rate. By subtracting the respiratory rate the second curve is obtained, which is the phytoplankton production rate. From this is subtracted the zooplankton grazing rate, yielding the curve at the bottom, which is the estimated rate of change of the phytoplankton.

- Riley used model to infer seasonal contributions of processes



Morel and Price (2003)
Trace metals and C, N, P
acquisition

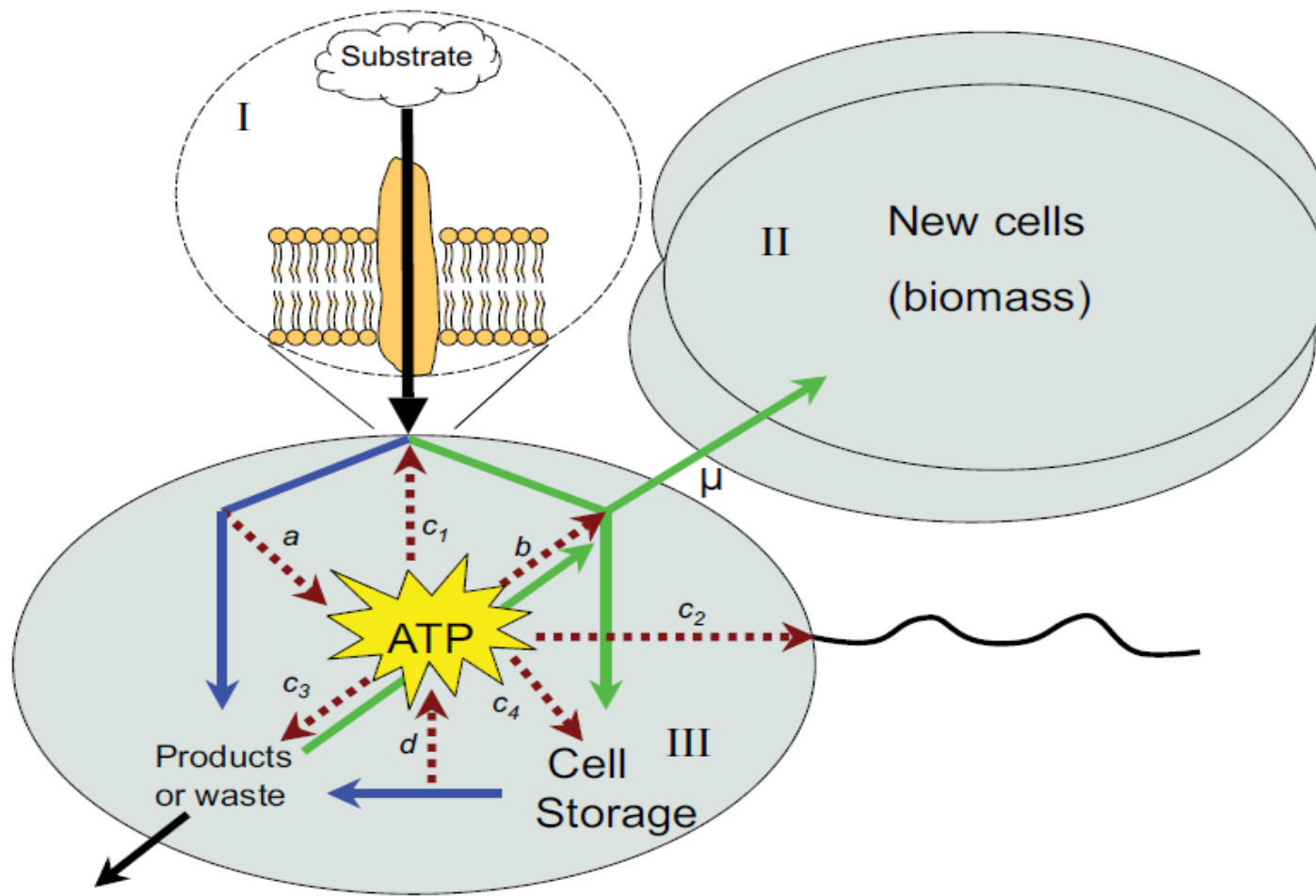


Figure 1. Substrate and energy flow within a cell. Substrate < 700 Da are actively taken up via membrane proteins (I). As the substrate enters the cell via active uptake, it either enters into catabolic pathways (blue lines) or anabolic pathways (green lines). Monomers for anabolism can come preformed from the environment or as products of catabolism. The red-hashed lines represent the flow of energy to and from these metabolic pathways. Energy is conserved via substrate catabolism and ATP is produced at a rate a . As ATP is hydrolyzed, energy is released and utilized at rate b to drive anabolic processes such as production of new cells (growth; II) and production cell storage products (III). Energy is also utilized at various rates to support processes that are independent of anabolism. This maintenance energy is used at rates c_1 to activate uptake systems, c_2 to fuel cell motility, c_3 to actively eliminate waste, and c_4 to repair cellular machinery. In the absence of exogenous organic substrates, the cell can yield ATP at rate d by catabolizing storage material (endogenous substrates). Adapted from del Giorgio and Cole (1998)

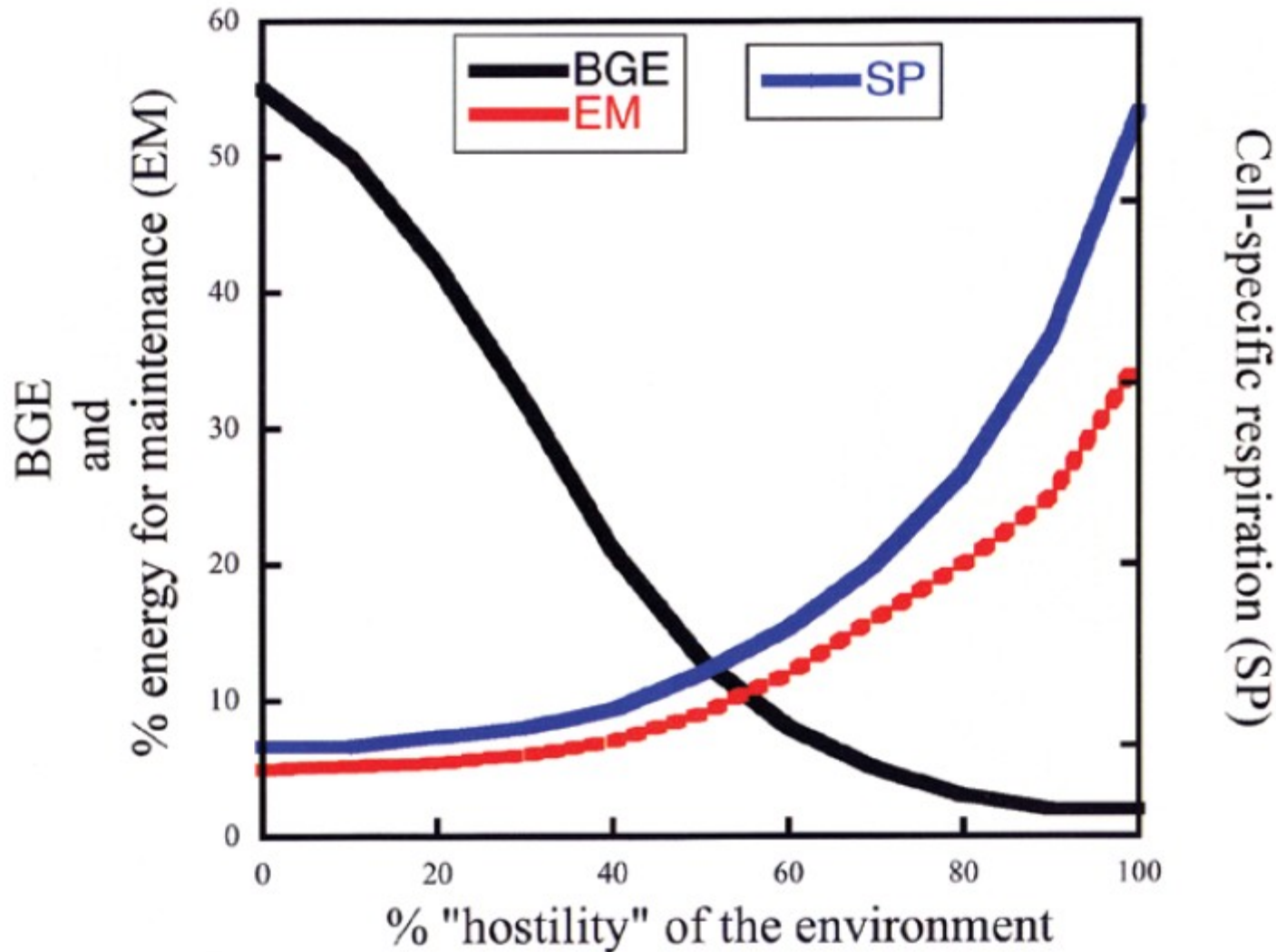


Figure 3. Conceptual diagram demonstrating the relationship between environmental stressors or environmental "hostility" and the partitioning of energy within a bacterial cell, the resulting bacterial growth efficiency (BGE), and cell specific respiration. As environmental hostility increases, more energy is partitioned into maintenance energy (EM). Thus, bacterial growth efficiency decreases and cell-specific respiration (SP) increases. Some combination of both physical (temperature, pH, salinity) and chemical (toxins, substrate availability) factors contribute to environmental hostility

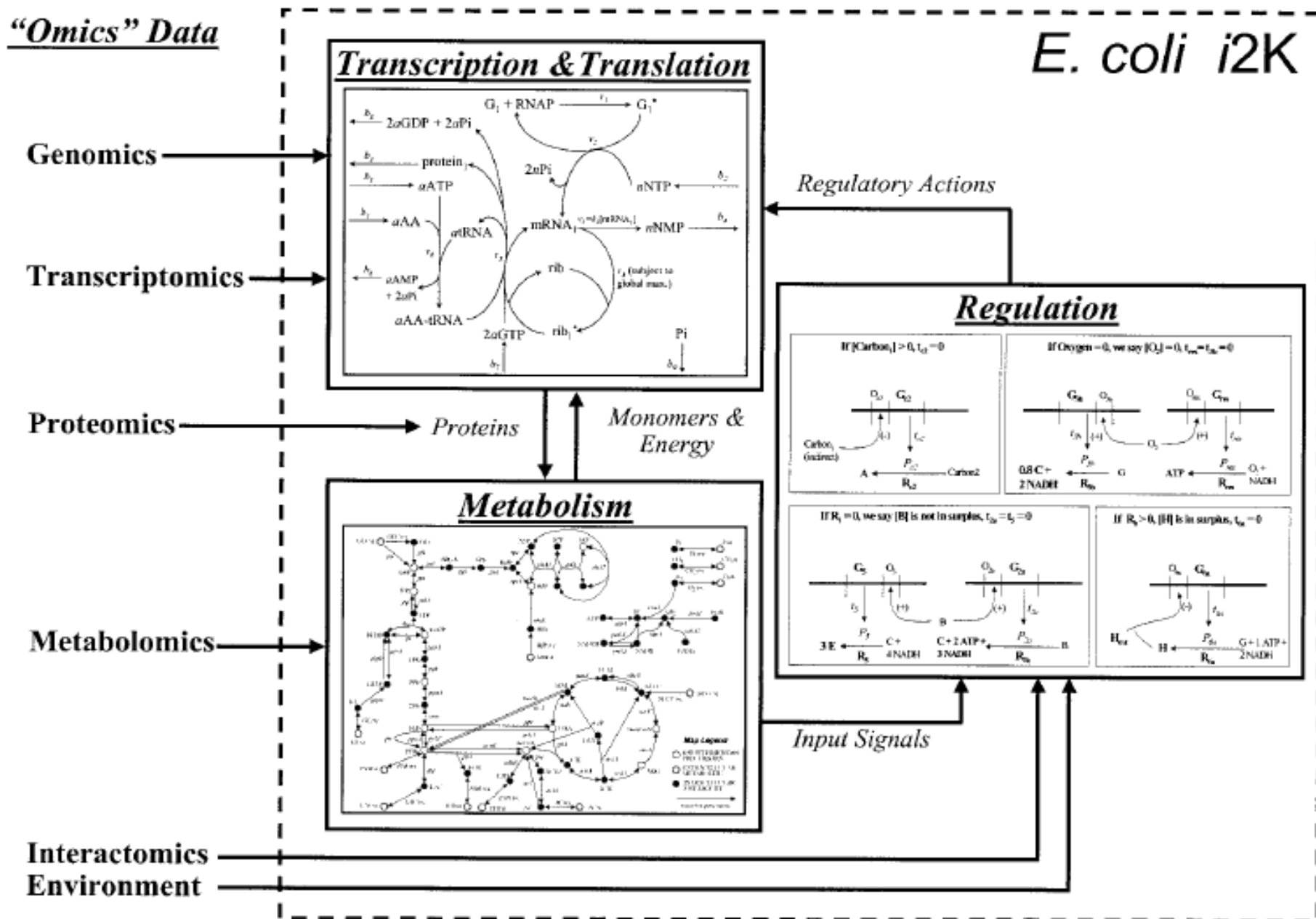
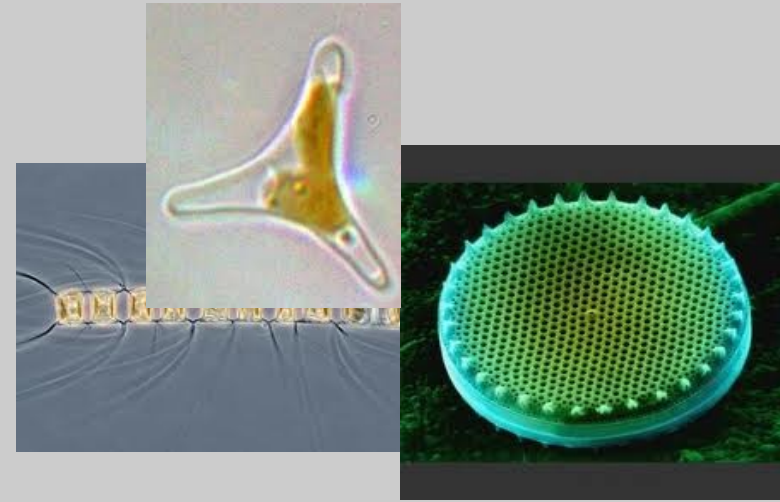


FIG. 4. Integrated constraint-based model of *E. coli*: the *E. coli* i2K model. Constraint-based modeling frameworks have been developed for metabolism (5, 14, 19, 50, 52, 62), regulation (9), transcription, and translation (1). The connectivity among the three modeling components is shown here. Integration of these three modeling components should produce an integrated model of *E. coli* that accounts for nearly 2,000 genes, referred to as the *E. coli* i2K model. This model can be used to reconcile diverse “-omics” data and utilize the data to more accurately predict a cellular phenotype.

Diatoms and Dinoflagellates

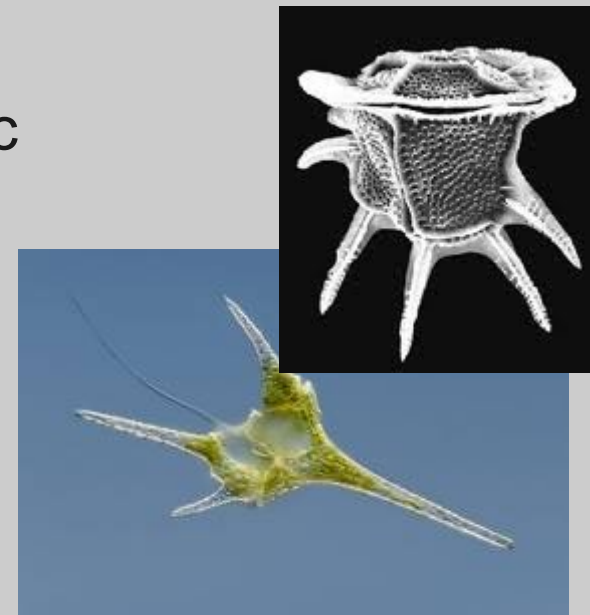
- Diatoms

- Photo-autotrophs
- Larger cells, spanning 5 – 500 microns
- Silica frustules
- Fast-growing opportunists



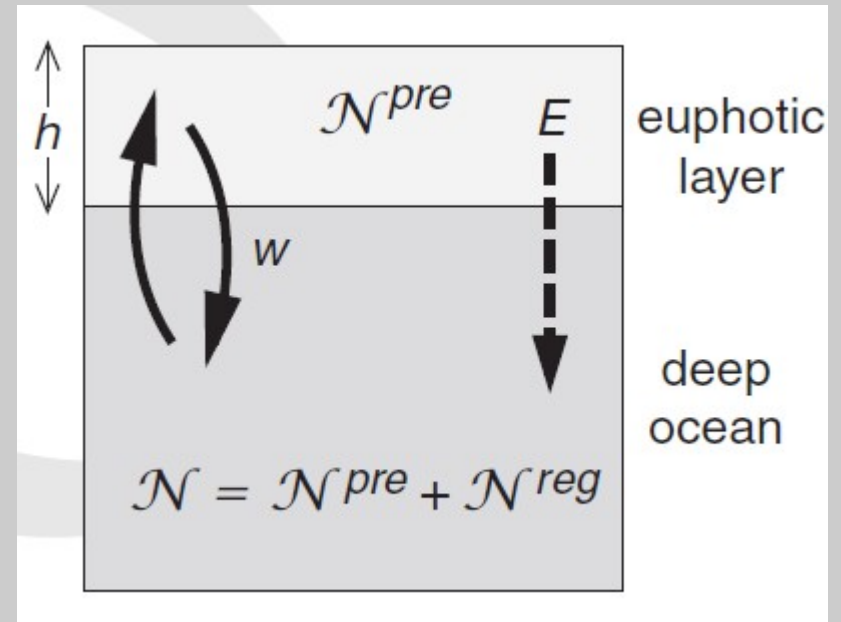
- Dinoflagellates

- Flagella
- Auto-trophic (?), mixotrophic and heterotrophic
- Large cells ~10's microns + (?)
- Slower growth rates
- Some produce toxins (Harmful Algal Blooms)

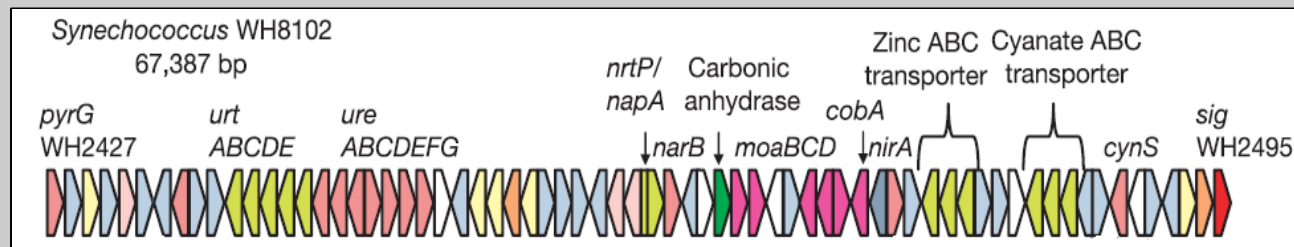


Ocean-Atmosphere Carbon Cycle

- Simple global model
- Highly parameterized
- Atmospheric $p\text{CO}_2$ function of export of organic carbon from surface and physical “flushing” of deep and surface waters.



$$\mathcal{P}^* = \frac{\mathcal{N}^{reg}}{\mathcal{N}} = \frac{E h}{w \{\mathcal{N}\}}$$



genome

Physiological information:
Mapping metabolic pathways

Ecological information:
Mapping environmental
distributions of ecotypes and
biogeochemical function

