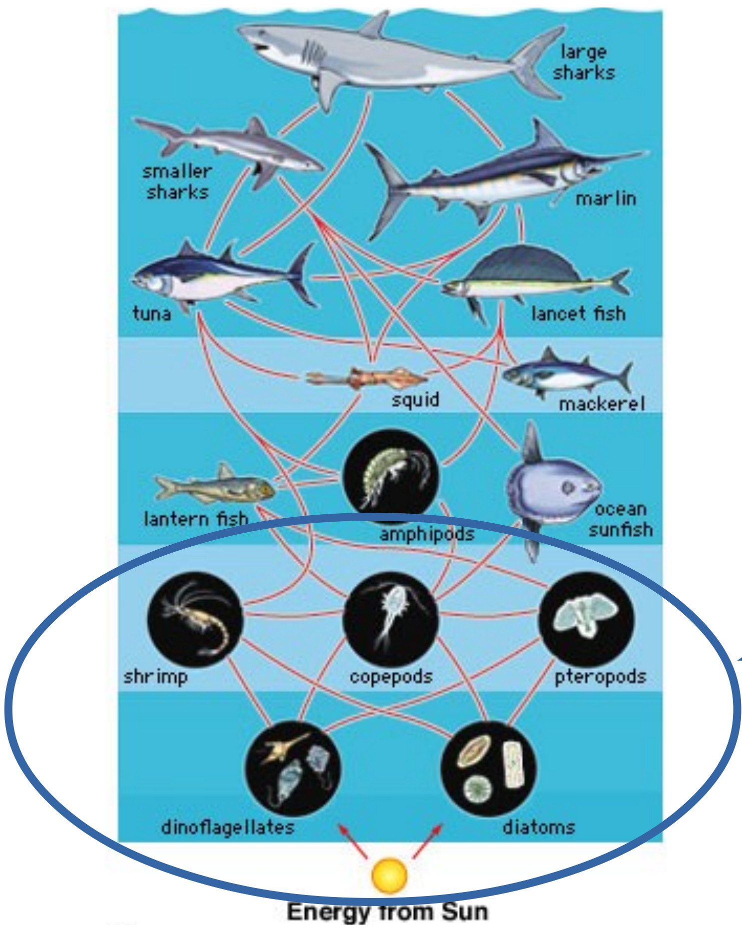
9 October 2023

Marine Ecosystem Modeling

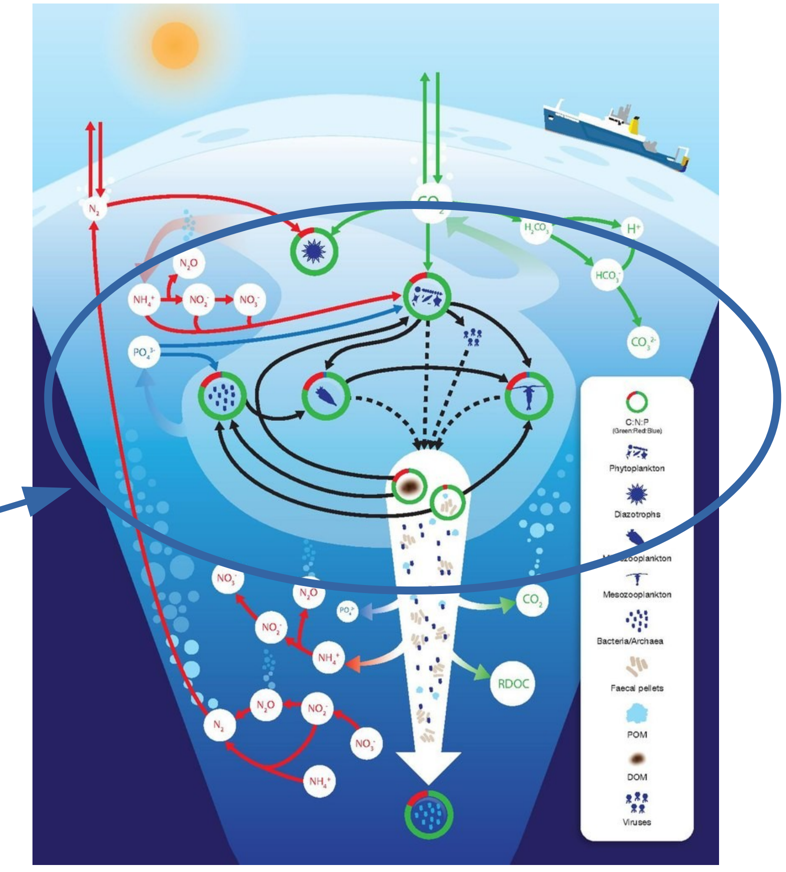
Beginners

Olivier Aumont, IRD-IPSL/LOCEAN, Paris, France

Some important restrictions



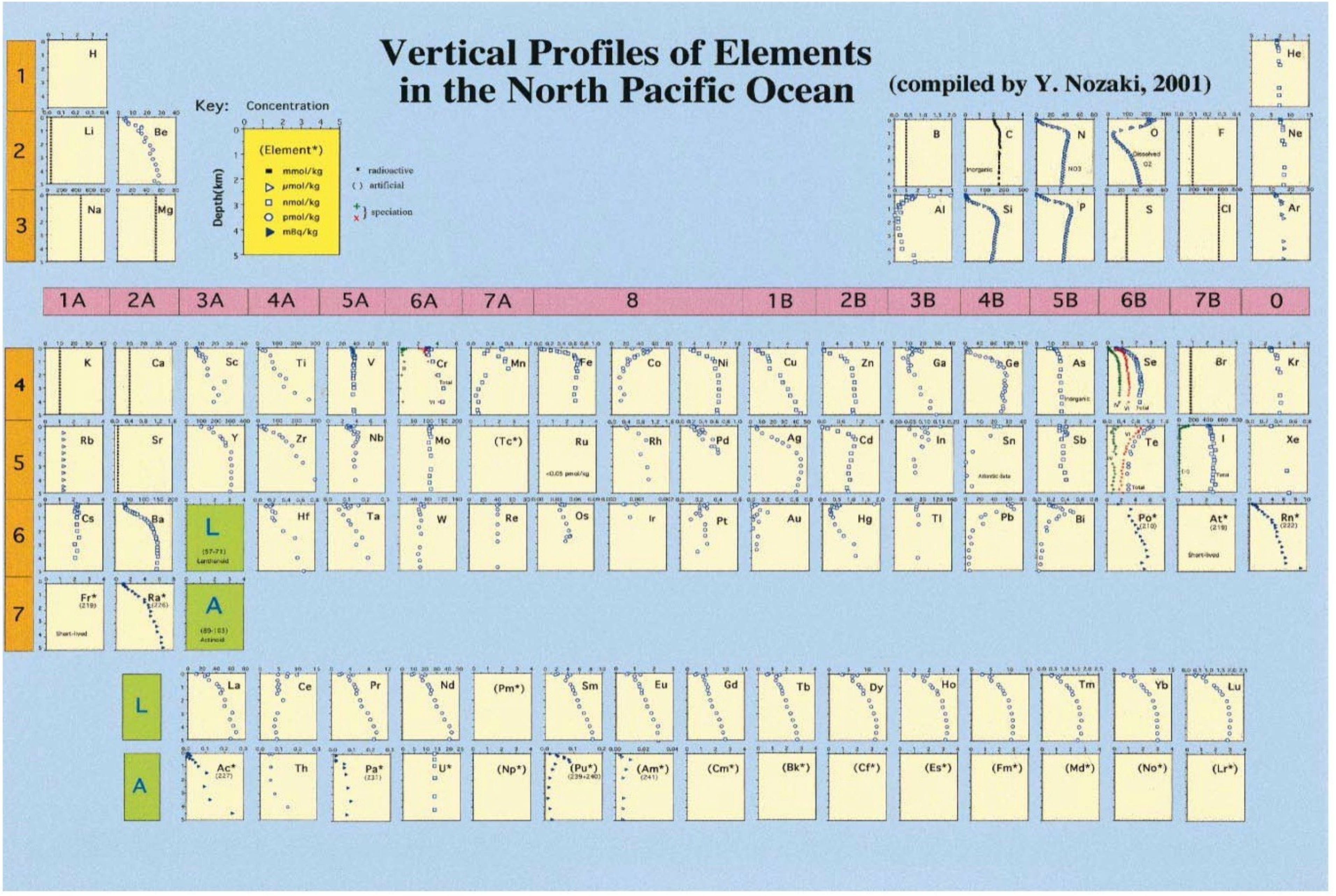
Ecosystem perspective



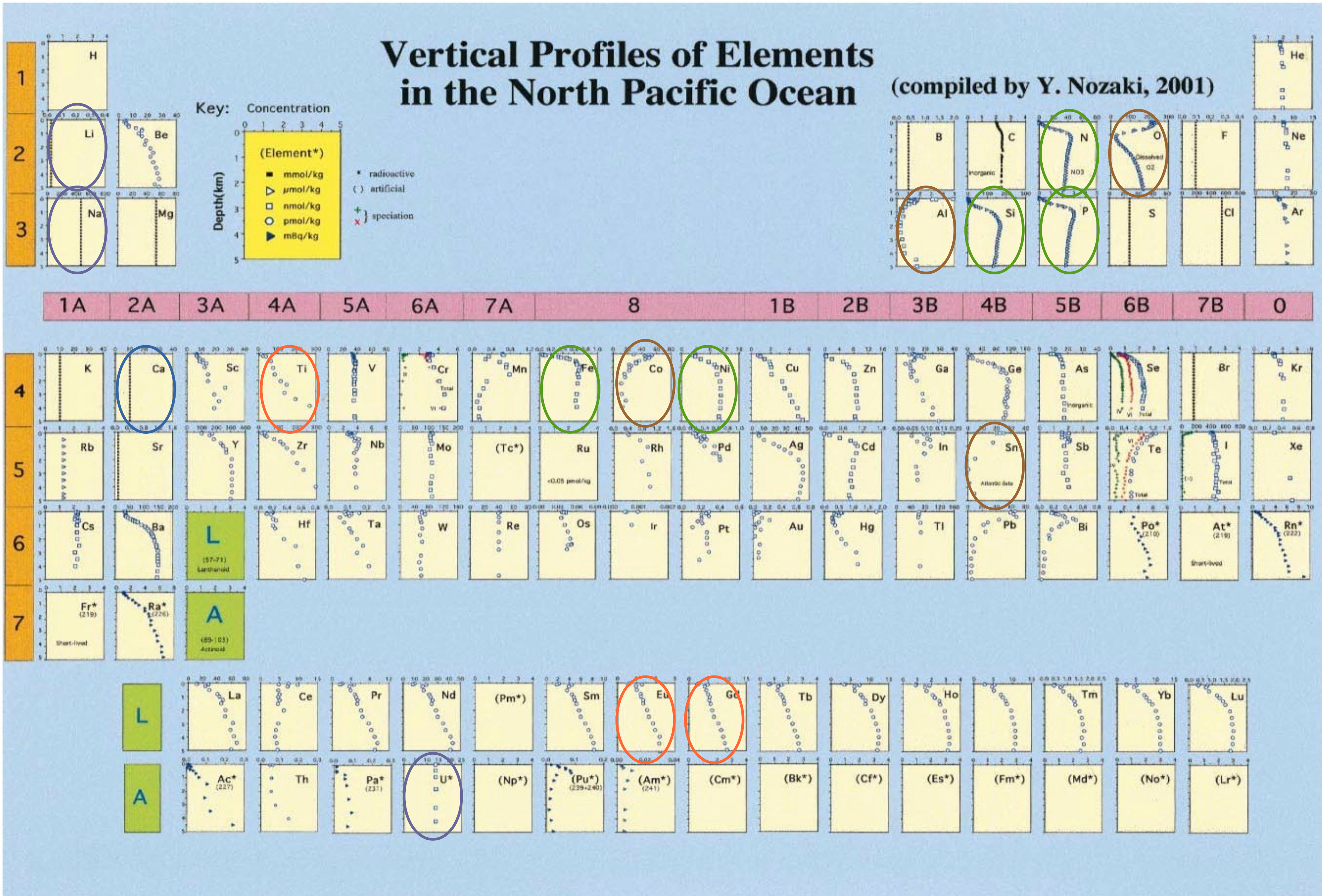
Biogeochemistry perspective

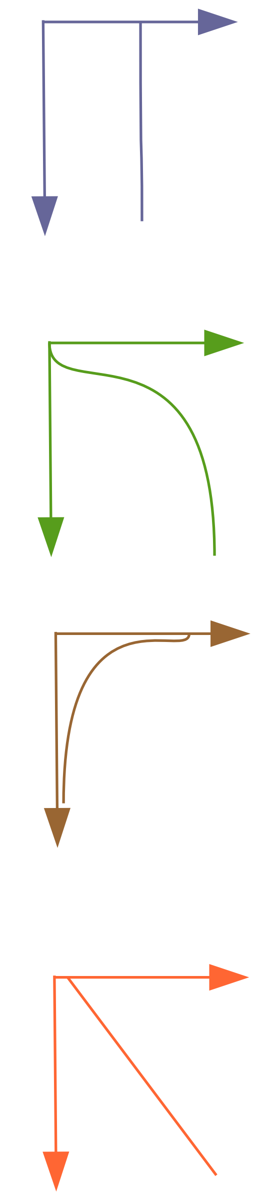
As a biogeochemist and a modeler, this presentation will be biased toward marine biogeochemical modeling and plankton ecosystems

Biogeochemistry in the ocean

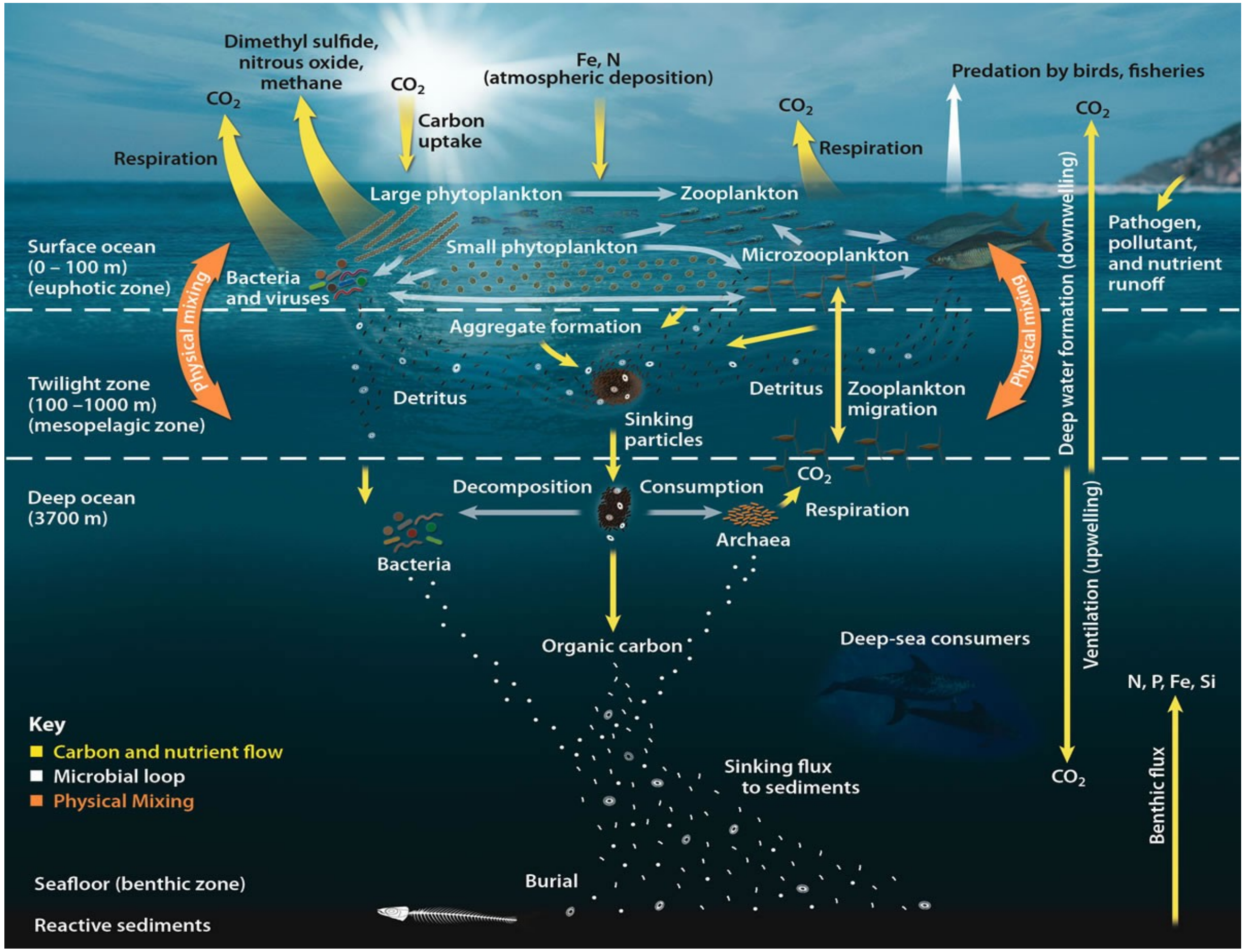


Chemical elements in the ocean: very diverse distributions





Marine biogeochemistry: numerous processes to consider



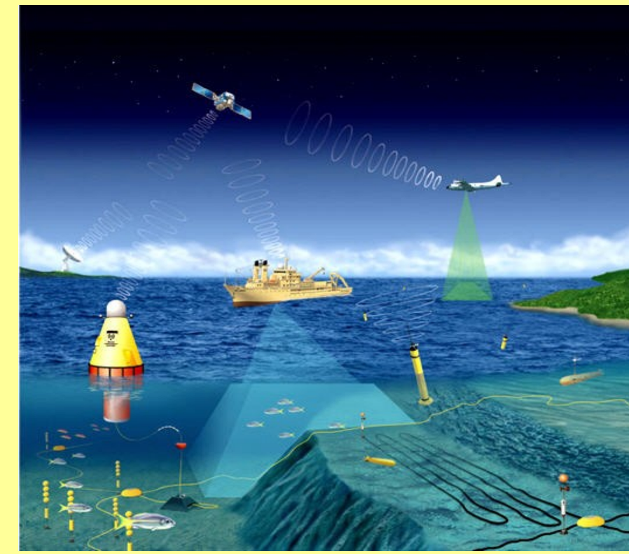
A great number of processes at play which are all coupled:

- Biological: photosynthesis, respiration, trophic interactions, …
- Chemical
- Physical: sedimentation, aggregation, mixing, transport, ...

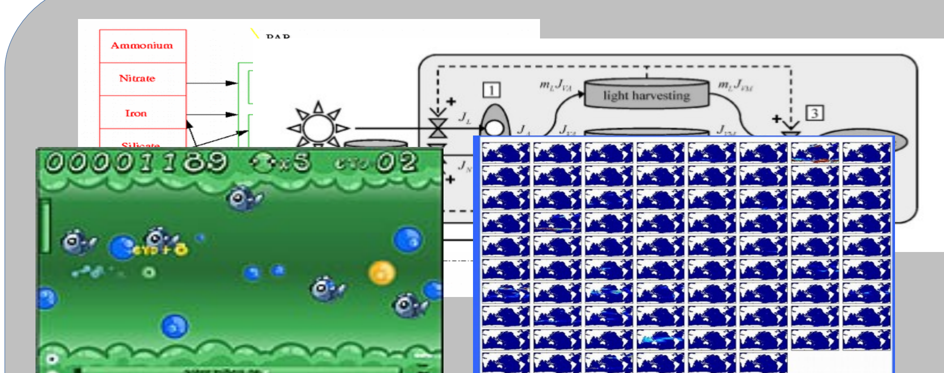
…

Observing and (hopefully) understand

Experiments in controlled environments



Observations



Modelling

Modeling: why?

- Hypotheses testing

  If we add, remove of change something, what happens?

- Quantitative dynamical framework

  Are some datasets and/or parameter estimates consistent?

- Assessing some unknown rates/parameters

  Based on observations, can we estimate some rates/fluxes/properties that are otherwise difficult to measure

- Prediction/forecasting

  What the ocean will look like at some point in the future (or in the (far) past)?

- Design of an observing system or campaign

  What is the best sampling strategy?

Overview of the presentation

- **Biogeochemical and ecosystem modeling: the different steps**

  Constructing a model

- An historical perspective

  When did it start and where we are

- Representing the physiology of the organisms

  The different ways to model the living compartments in a model

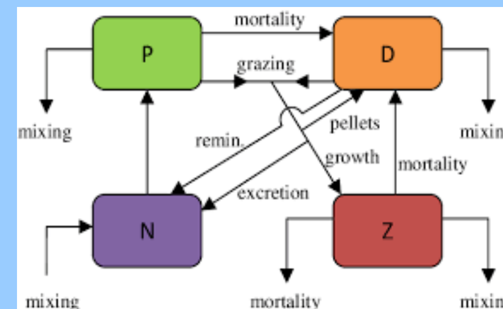
- Modeling functional biodiversity

  PFT models, trait-based models, gene-centric models, ...

- Final words

Modeling: what does it mean?

Observations, functional constraints, ...

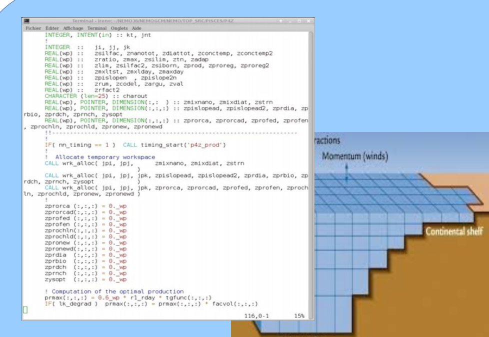


Formalism: what do we model and how ?

$$\frac{\partial DIN}{\partial t} = -\overbrace{V_m f(I) \left[\frac{DIN}{K_u + DIN}\right] P}^{f_{np}} + \overbrace{\Xi P}^{f_{pn}} + \overbrace{\Gamma Z + R_m \gamma \left[1 - e^{-\Lambda P}\right] Z}^{f_{zn}}, \qquad (A1)$$

Mathematical model

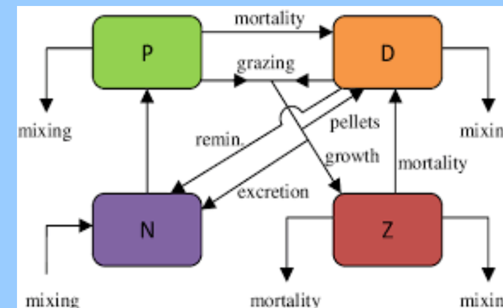
Running, debugging, tuning, optimizing



Coding and numerics

Modeling: what does it mean?

Obervations, functional constraints, ...



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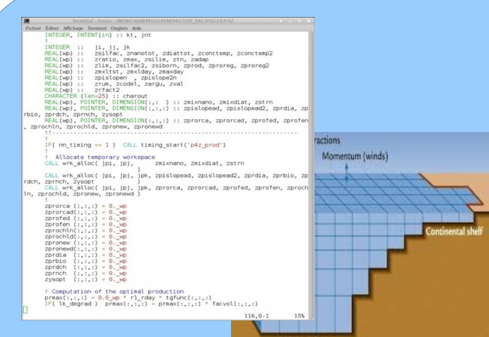


Coding and numerics

Mass conservation in a fluid

Relevant for nutrients and planktonic organisms

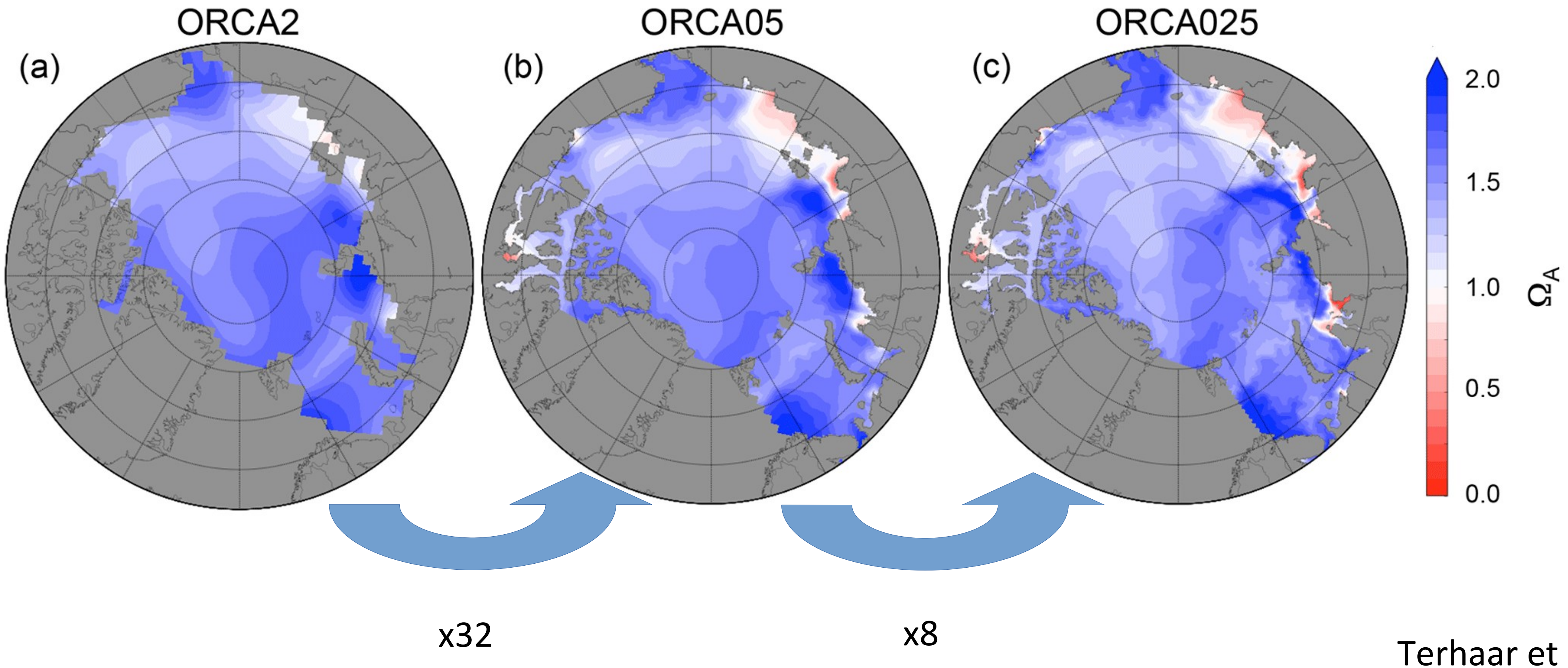
$$\frac{\partial C}{\partial t} = \underbrace{-C\nabla\vec{v}}_{\text{Advection}} + \underbrace{\frac{\partial}{\partial z}K_z\frac{\partial C}{\partial z}C + \nabla_h\cdot\left(K_h\nabla_h C\right)}_{\text{Diffusion (non resolved processes)}} + \underbrace{SMS}_{\text{Biogeochemical Sources and Sinks}}$$

- **Modeling ocean biogeochemistry and (planktonic) ecosystems requires an ocean circulation model**
- Any biases in the simulated ocean dynamics produce biases in marine biogeochemical and ecosystem models
- All the challenges related to dynamical modeling are pertinent for ocean biogeochemical modeling

  Mesoscale/submesoscale, Mixing, overflows, boundary layers, ...

A first challenge: The computing cost

- Better modeling of the ocean circulation (and of the environment) generally requires to increase the spatial resolution
- Better modeling of the ecosystem and biogeochemical processes generally requires to increase the number of processes and prognostic variables (tracers)



Terhaar et al., 2019

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Ecosystem/biogeochemical modeling: an historical perspective

- The pioneering studies : date back to the middle of the XXth century
- The first marine ecosystem model : Fleming (1939)

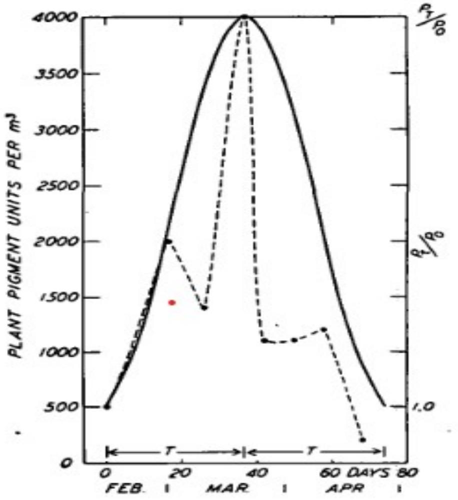
The Control of Diatom Populations by Grazing.*)

By

Richard H. Fleming,

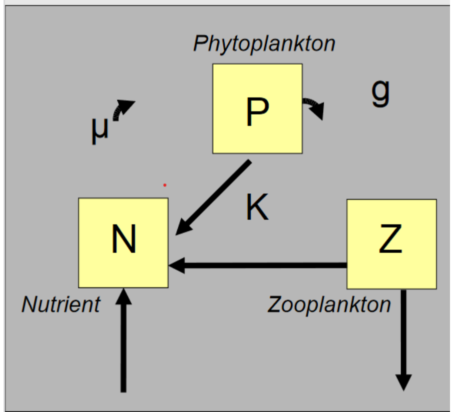
Scripps Institution of Oceanography, University of California, La Jolla, California.

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



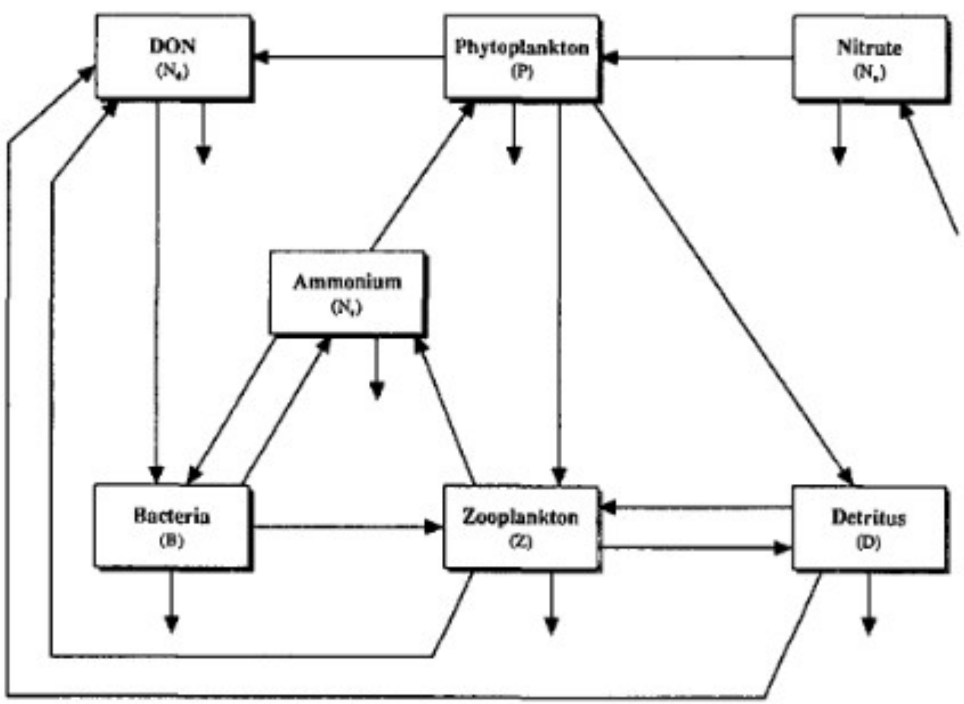
Simulation of a diatom bloom in the Channel

- The first NPZ-type model coupling the dynamics of nutrients, phytoplankton and zooplankton: Steele (1974)



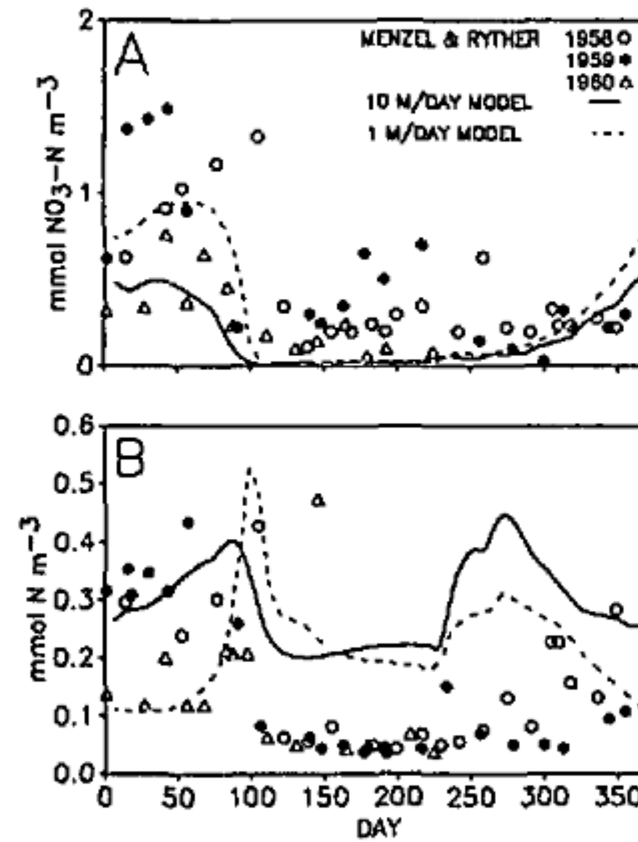
Ecosystem/biogeochemical modeling: Fasham et al. (1990)

- They defined the structure and the formulation of NPZD-type models on which most existing biogeochemical/ecosystem models currently rely



NO3

P



- All studies were restricted to 0-D or quasi 0-D frameworks

Spatially resolved biogeochemical models

Geochemical

PO_4^{3-}

Particles

Euphotic Layer (100-150m)

→ A single equation for the whole « biology » :

export production = f(Temp) . f(light) . PO_4^2 / (Ks+PO_4)

→ The simplest models used in the global ocean models

HAMOCC (1990)

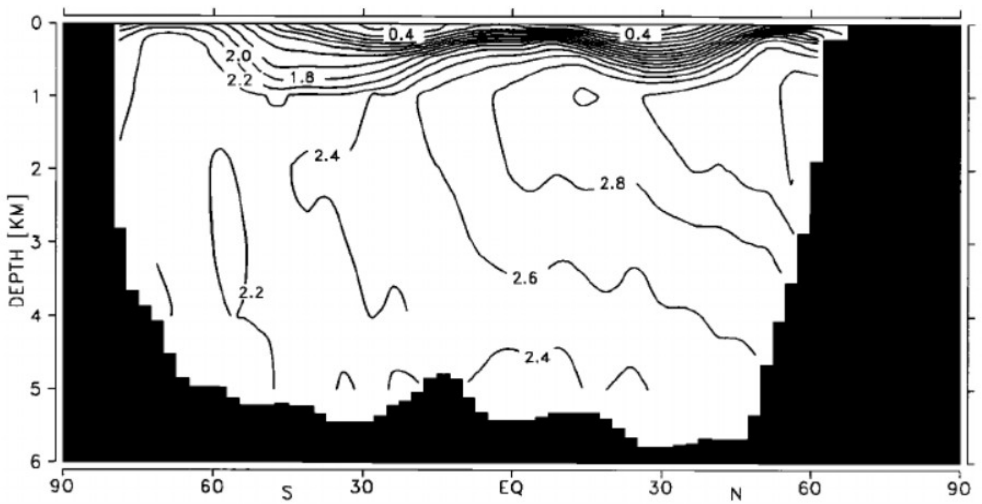
How were they performing?

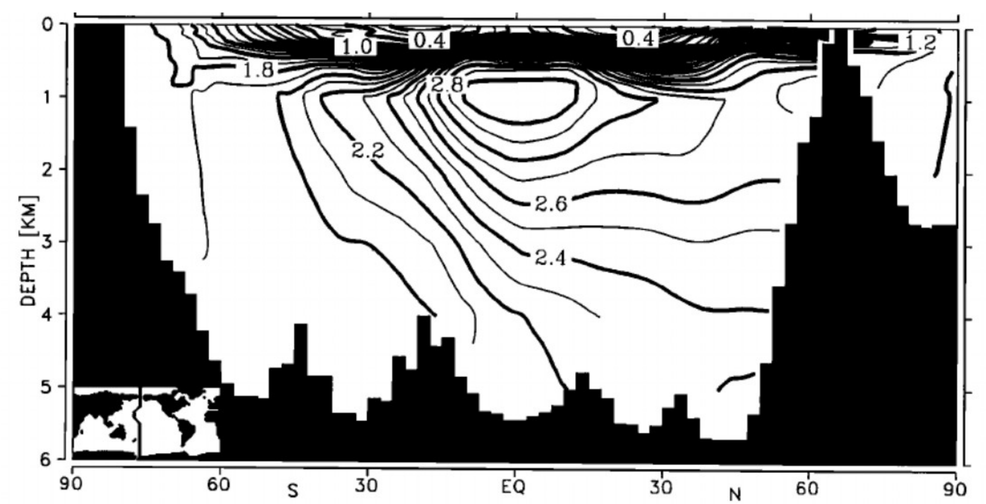
- They were extremely cheap but that was necessary considering the computing power available at that time

- Long-term simulations were feasible (paleo, future, steady-state)

- They were doing a decent job at reproducing the large-scale annual-mean patterns

Phosphate distribution in the Pacific ocean



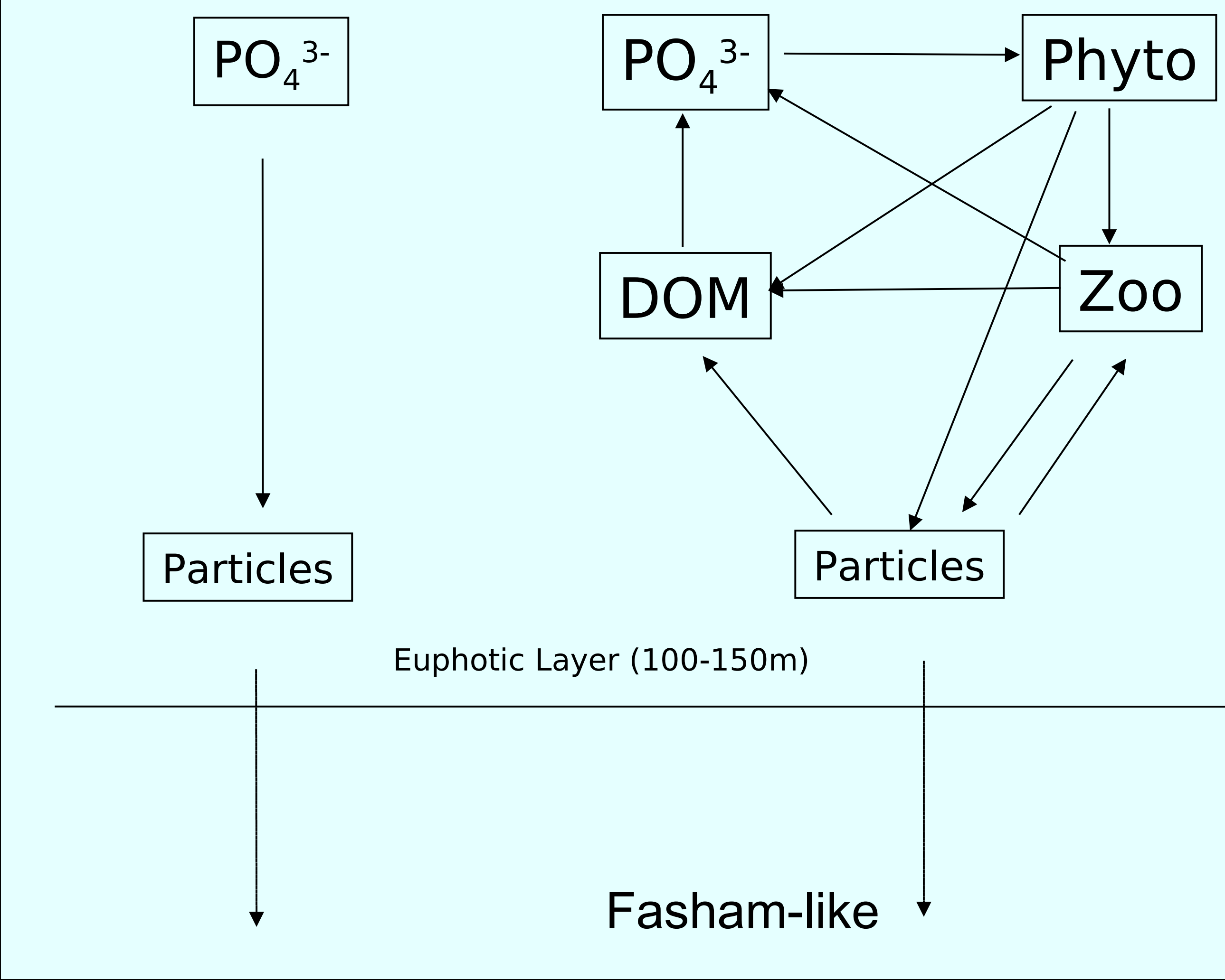


- Current models perform better, but not by a lot and a large part of the improvement comes from a better representation of ocean dynamics

The first large-scale ecosystem (biogeochemical) models

Geochemical

NPZD



GLOBAL BIOGEOCHEMICAL CYCLES, VOL. 7, NO. 2, PAGES 417-450, JUNE 1993

A SEASONAL THREE-DIMENSIONAL ECOSYSTEM MODEL OF NITROGEN CYCLING IN THE NORTH ATLANTIC EUPHOTIC ZONE

J. L. Sarmiento,[1] R. D. Slater,[1] M. J. R. Fasham,[2] H. W. Ducklow,[3] J. R. Toggweiler,[4] and G. T. Evans [5]

GLOBAL BIOGEOCHEMICAL CYCLES, VOL. 10, NO. 4, PAGES 559–583, DECEMBER 1996

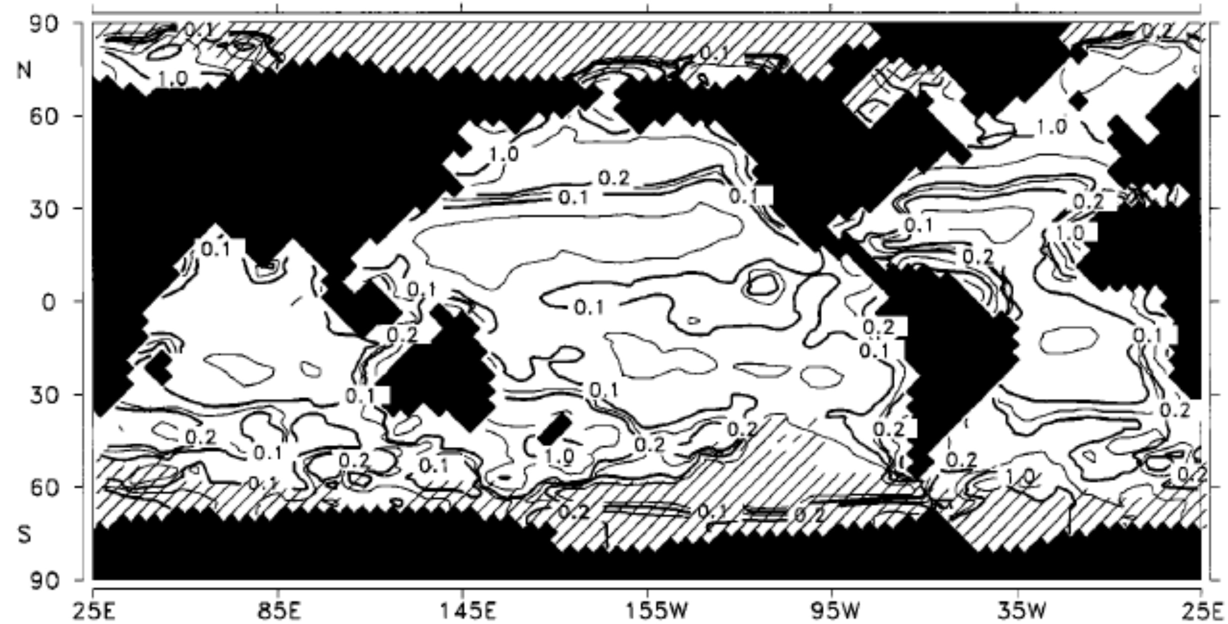
Effects of plankton dynamics on seasonal carbon fluxes in an ocean general circulation model

Katharina D. Six and Ernst Maier-Reimer
Max-Planck-Institut für Meteorologie, Hamburg, Germany

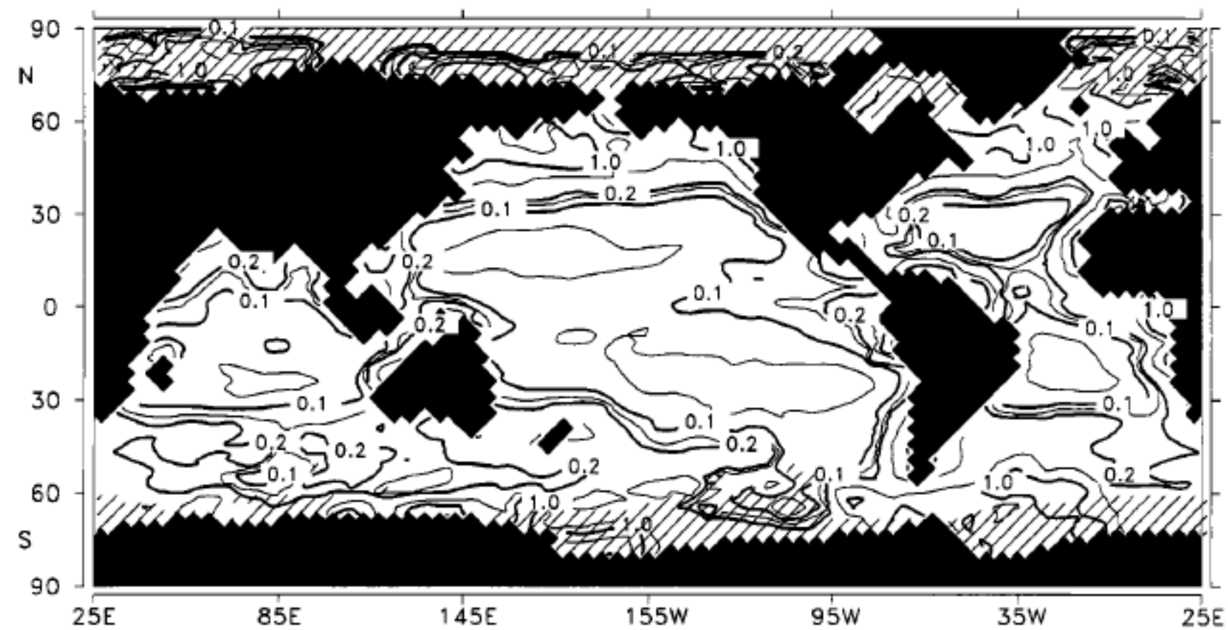
An example

Annual-mean surface Chl (mg Chl/m^3)

Satellite

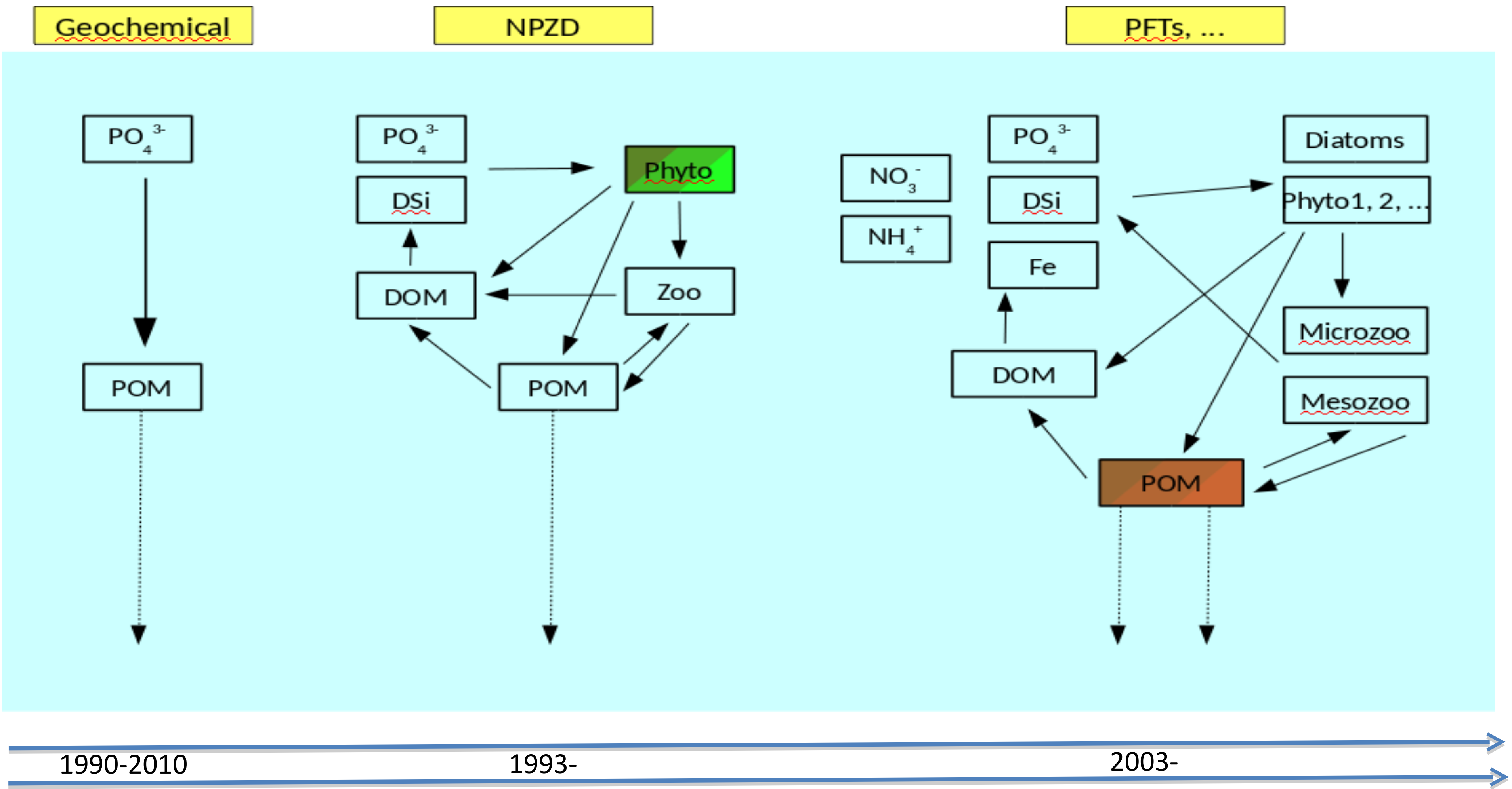


HAMOCC3.1



Six and Maier-Reimer (1996)

Models have become more and more complex

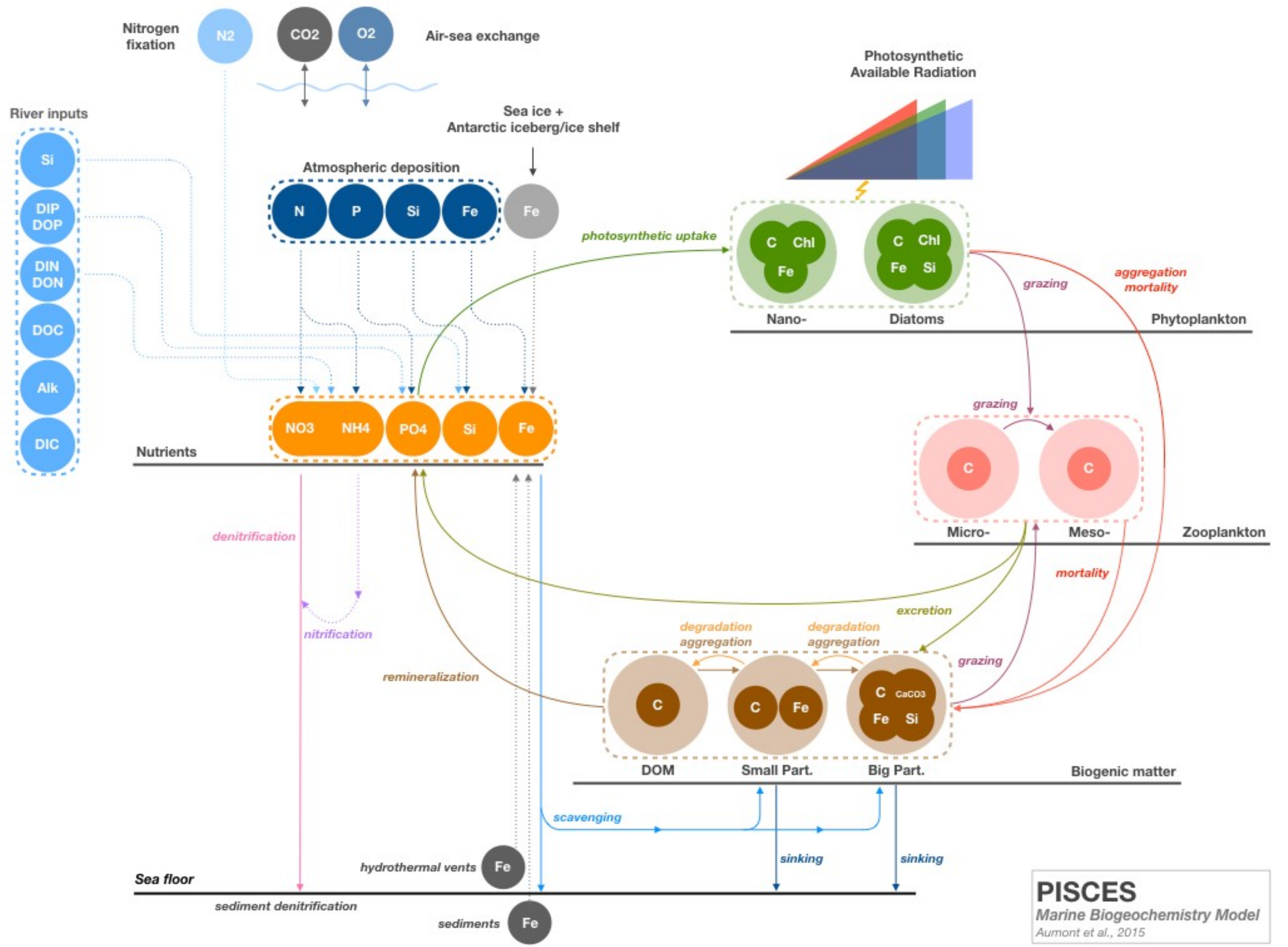


- More complex does not necessarily imply more realistic! (Anderson, 2005; Friedrichs et al., 2007; Ward et al., 2013)

- A huge set of (often) badly constrained parameters

PISCES: An example of a (quite) complex ecosystem/biogeochemical model

- 24 tracers
- ~100 parameters

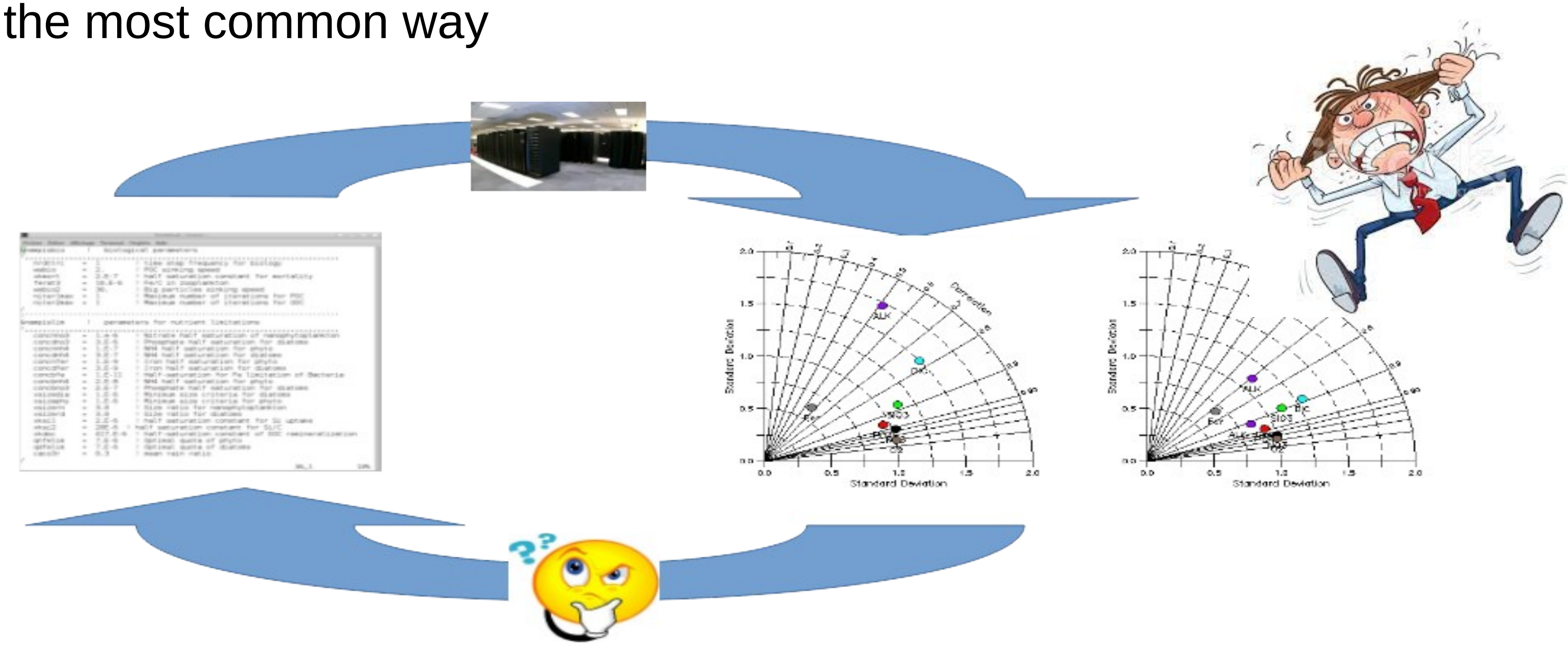


Aumont et al., 2003 ; Aumont et Bopp, 2006 ; Aumont et al., 2015

A second challenge: tuning/evaluating the models

- Hand tuning: the most common way

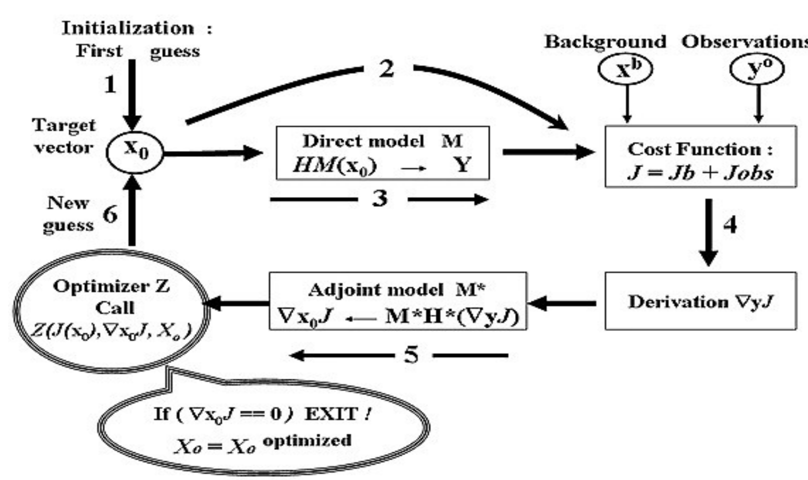
10, 20, 100x, ...



We learn a lot from the model dynamics (intuitive knowledge)

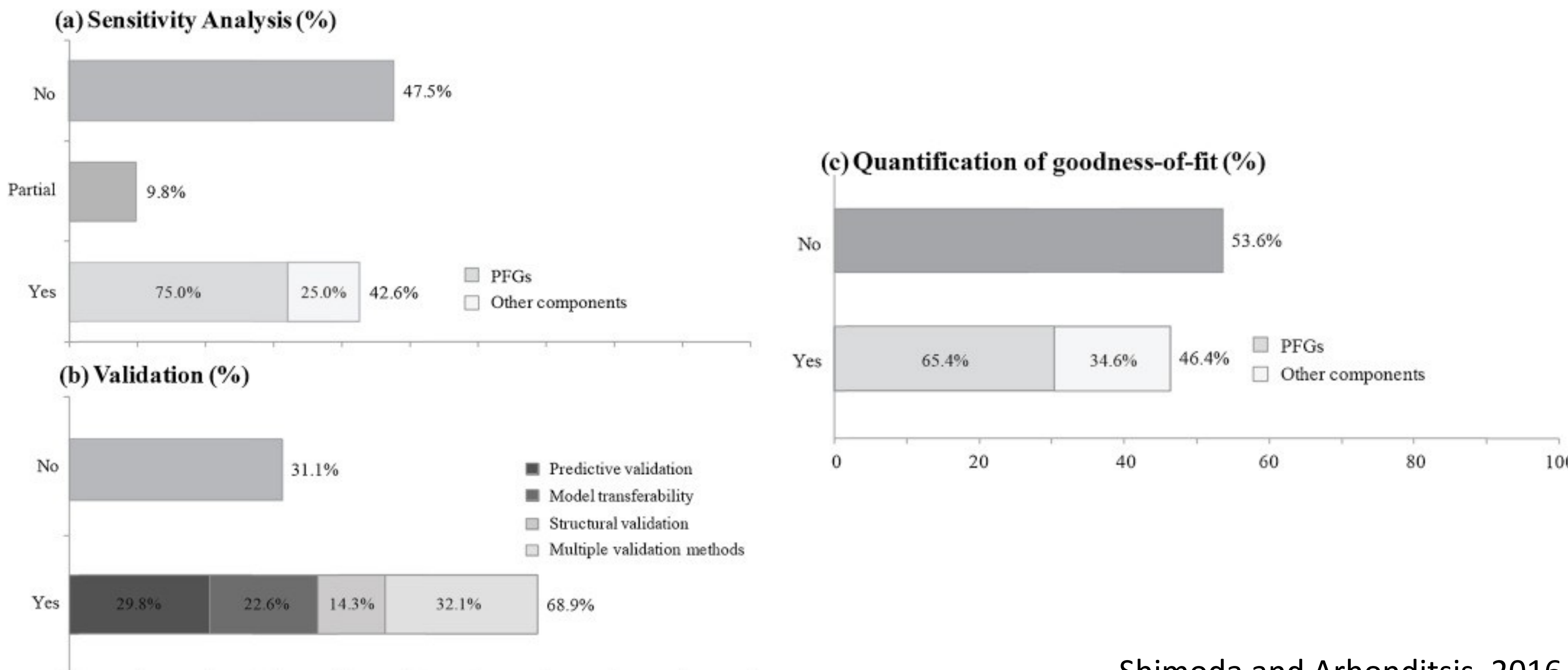
- Data assimilation approaches

Numerous difficulties



A second often hidden challenge

- Quite surprisingly, this step is often overlooked or not reported, despite it is a critical step



Shimoda and Arhonditsis, 2016

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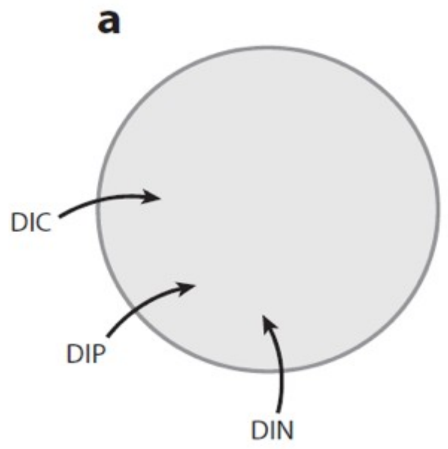
Modeling cell physiology



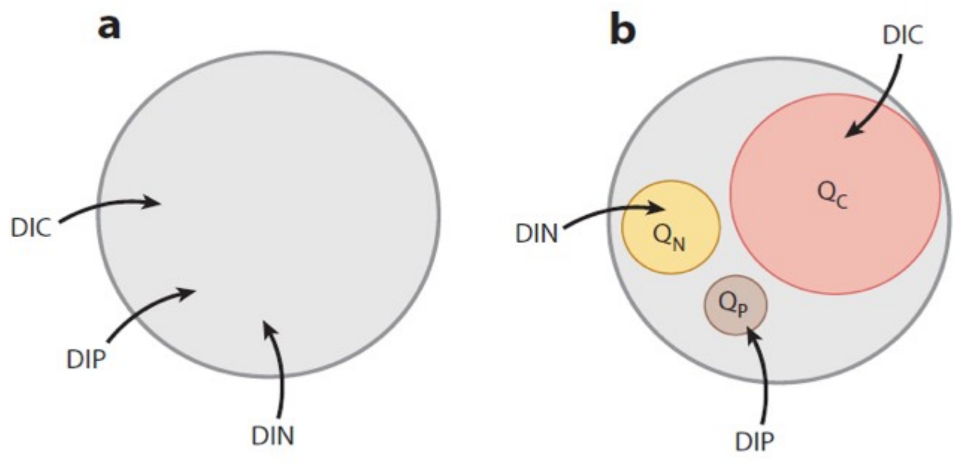
$$\frac{dP}{dt} = \mu_{max} * \frac{N}{K_N + N}$$

1940s

Monod/
Redfield

1 tracer/ pool

Modeling cell physiology

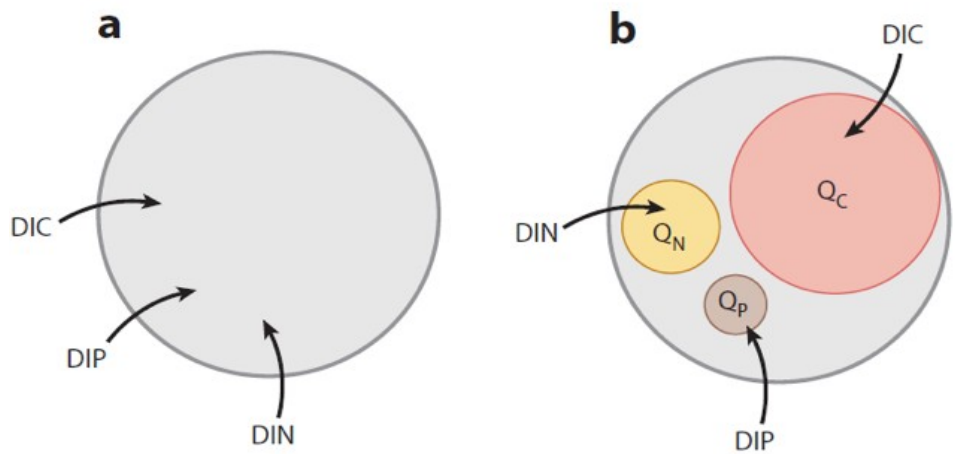


$$\frac{dQ_N}{dt} = V_{max} \frac{N}{K_N + N} - \mu Q_N$$

$$\frac{dP}{dt} = \mu_{max} * \left(\frac{1 - \frac{Q_{min}}{Q_N}}{1 - \frac{Q_{min}}{Q_{max}}} \right) P$$

1940s	1960s
Monod/ Redfield	Droop/ Caperon Internal stores
1 tracer/ pool	2/5 tracers/ pool

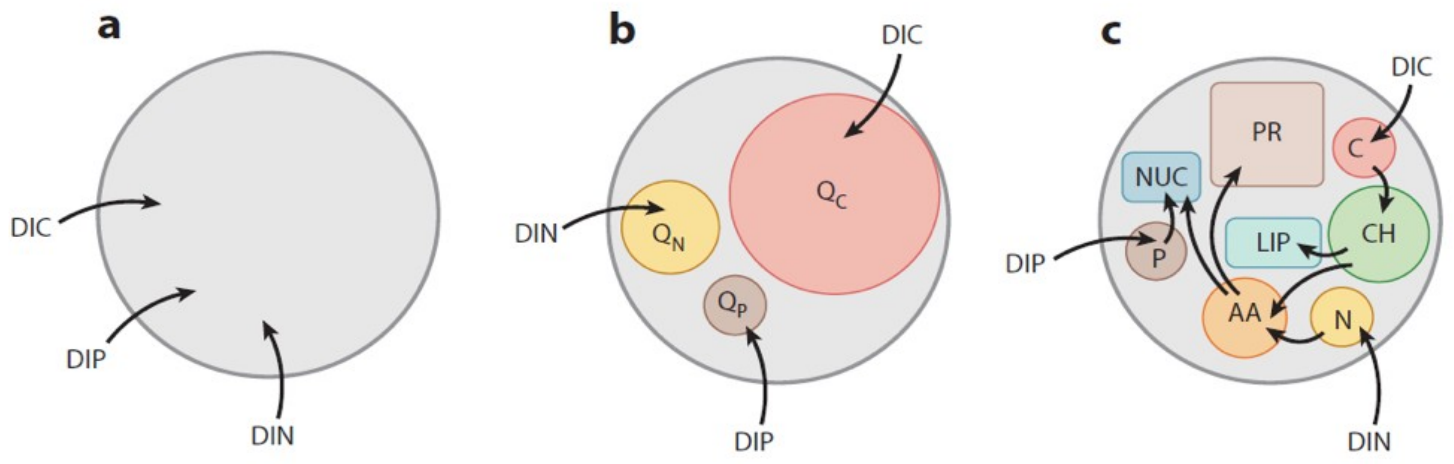
Modeling cell physiology



Most biogeochemical/ecosystem models belong to one or the other of these classes

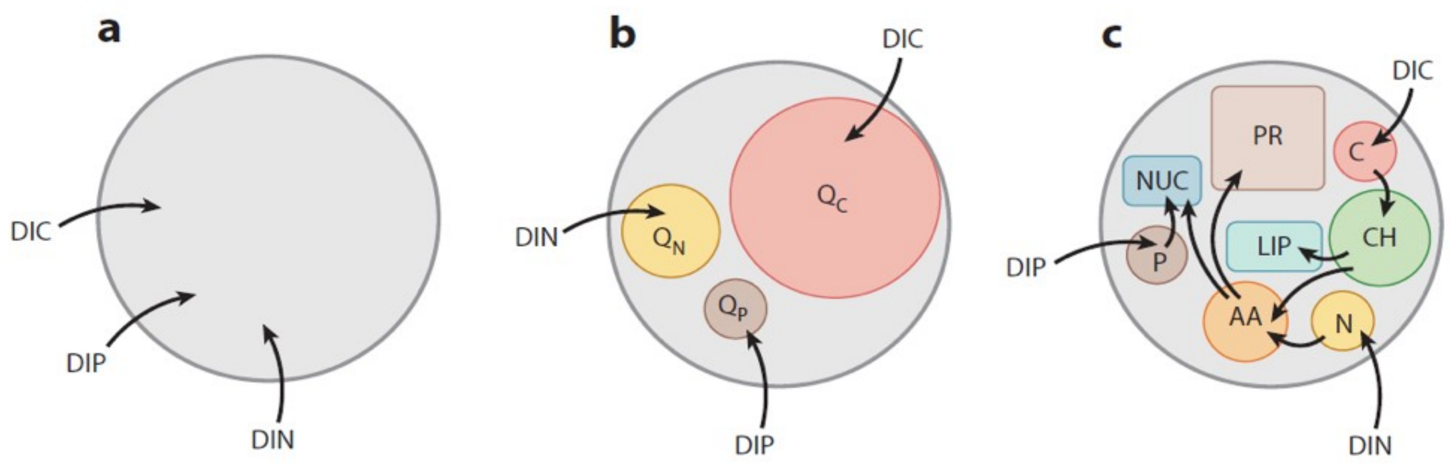
1940s	1960s
Monod/ Redfield	Droop/ Caperon Internal stores
1 tracer/ pool	2/5 tracers/ pool

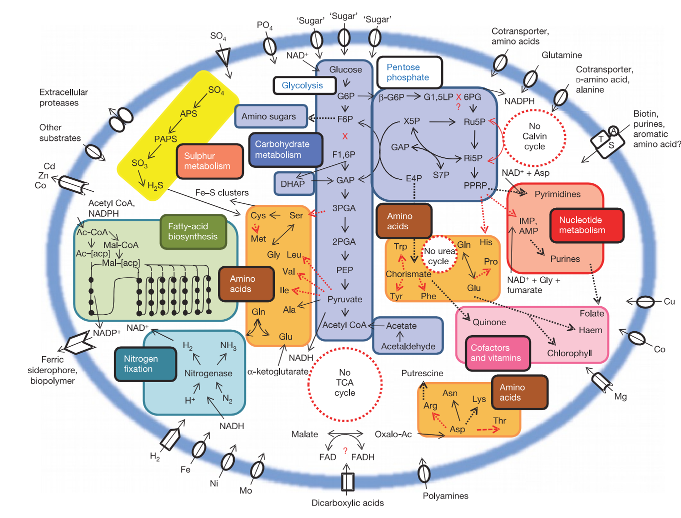
Modeling cell physiology



1940s	1960s	1970s
Monod/ Redfield	Droop/ Caperon Internal stores	Shuter, Shuler Macro-molecular models
1 tracer/ pool	2/5 tracers/ pool	~10 tracers/ pool

Modeling cell physiology

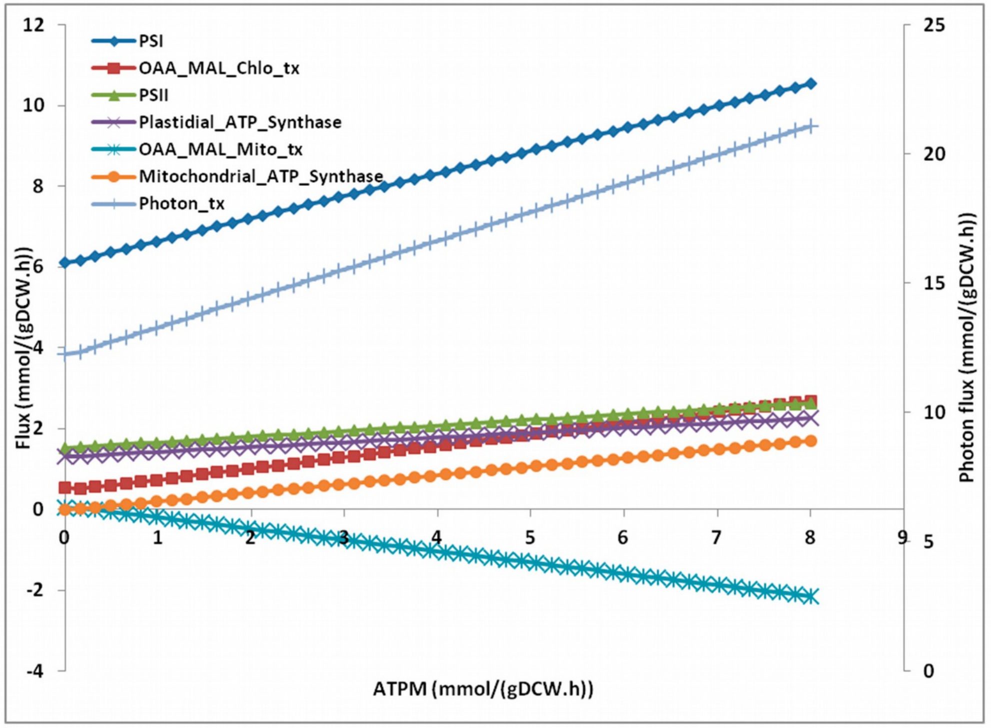




1940s	1960s	1970s	2000s
Monod/ Redfield	Droop/ Caperon Internal stores	Shuter, Shuler Macro-molecular models	Metabolic Reconstruction FBA
1 tracer/ pool	2/5 tracers/ pool	~10 tracers/ pool	~100-1000 tracers/ pool

- Very promising, for instance to evaluate the benefits and costs of metabolic pathways
- Identification of new metabolic pathways

Difficulties



Simulated effect of variations in ATPM on metabolism in a diatom

Ahmad et al. (2020)

- Not feasible considering the current computational constraints. Needs coarse-grained techniques
- This level of information is not available for most organisms
- FBA approaches assume steady-state or successive quasi steady-states (dFBA)
- Requires to specify an objective function to optimize which is not always easy

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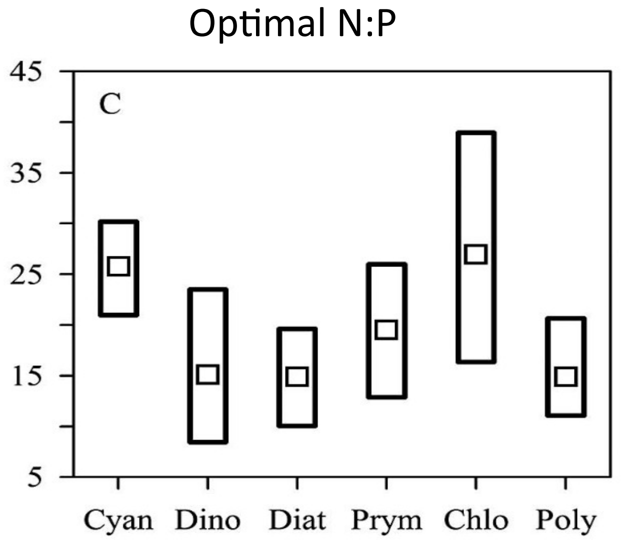
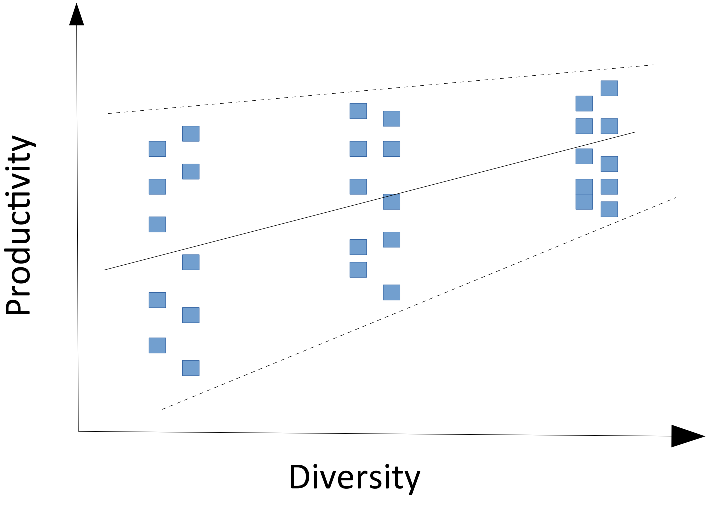
Modeling (functional) biodiversity

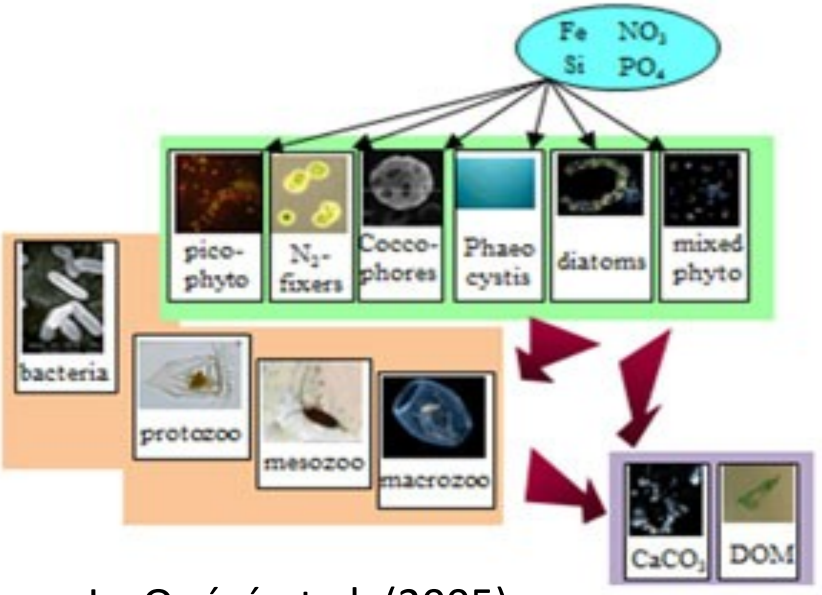
- A great challenge for biogeochemical/ecosystem modeling is to represent biodiversity
- Biodiversity = functional biodiversity
- Biodiversity has important consequences on biogeochemistry and ecosystem functioning



Hillebrand et al. (2013)



Plankton Functional Types Models



Le Quéré et al. (2005)

- **How to define PFTs?**

A PFT should have a specific biogeochemical/ecosystem function

A PFT could be allocated a distinct set of physiological /environmental/food/… characteristics

A PFT should have some importance in a region of the ocean

- **Difficulties**

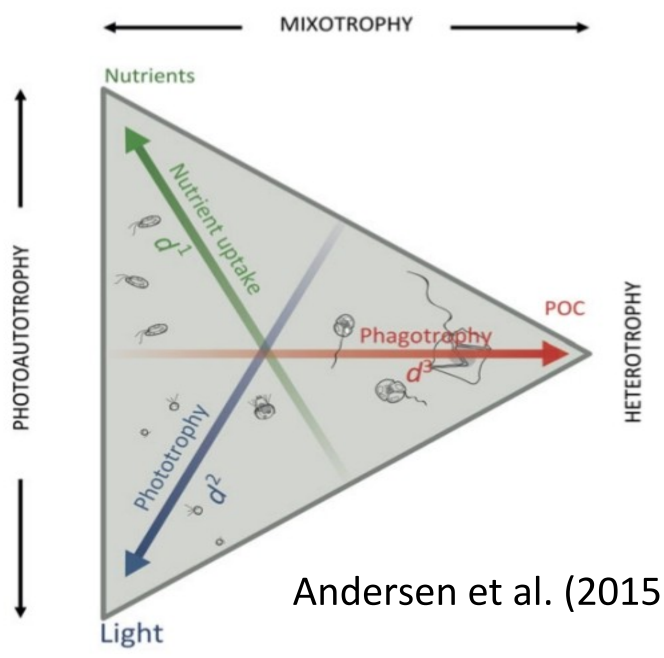
Numerous species are lumped into a limited number of boxes

How many boxes should be set? How to set a single set of parameters?

Fixed, a priori-defined structure of the model

Tuning becomes quickly a pain!

Trait-based models



Andersen et al. (2015)

- **What is it?**

Species are not specifically modeled

Organisms are identified by a few taxa-transcending properties: their key traits and the trade-offs between them

Structure and function of ecological communities emerge from properties of the individual organisms.

- **Difficulties**

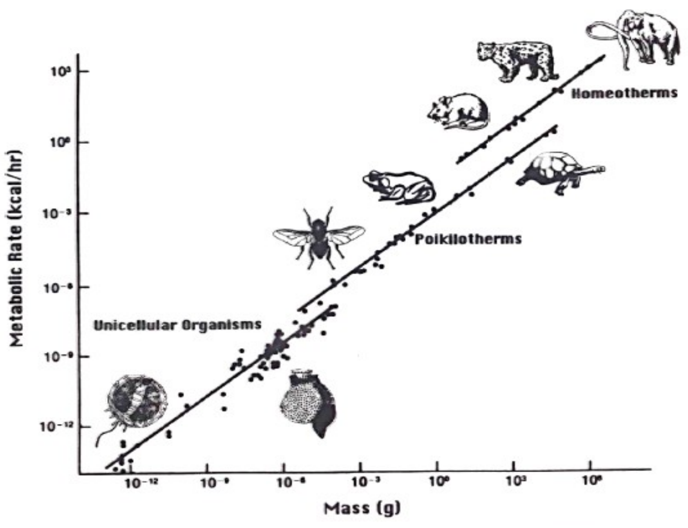
What traits should be represented?

Quantifying the trade-offs is very often challenging. Metabolic reconstruction can be very promising.

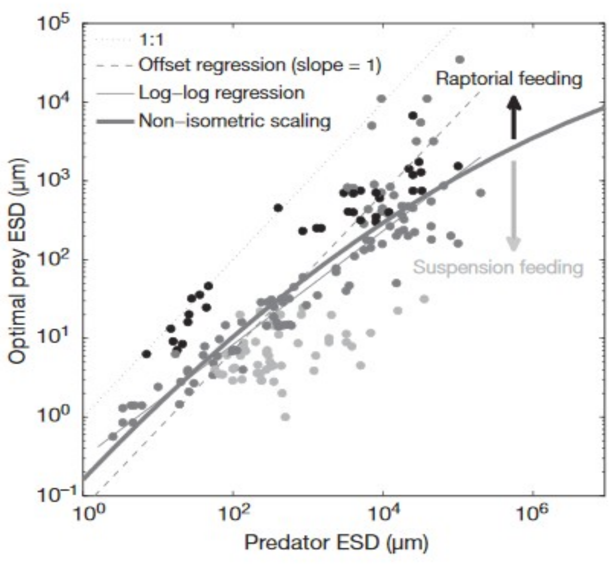
All traits are (most of the time) accessible everywhere/all the time. Evolution?

Can be very very expensive (1 trait = 1 additional dimension to the problem)

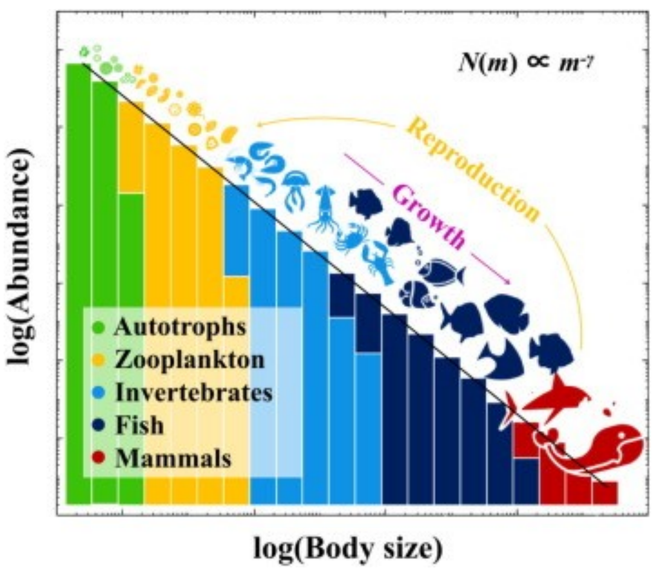
Size is a master trait



- Many metabolic rates show some dependency to size (allometry) $Y = Y_0 W^b$
- Many processes/fluxes are impacted by size: sinking of particles, feeding strategy, motility, vertical migrations, …
- Trophic interactions are influenced by size (who's eating whom?)
- Biomass distribution as a function of size often shows some regular properties (Sheldon et al., 1972)



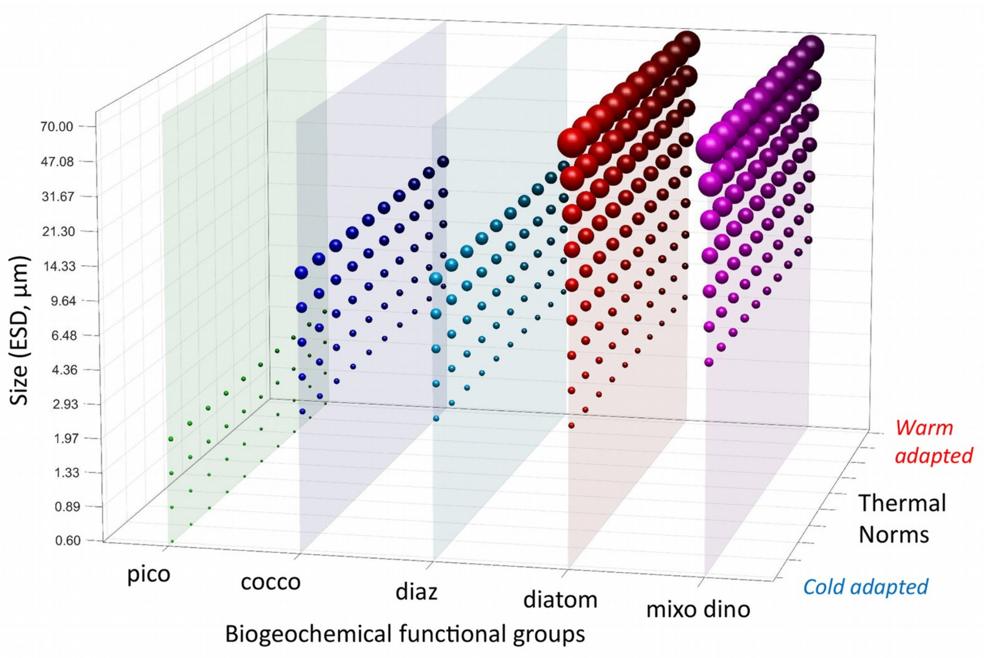
Wirtz (2012)

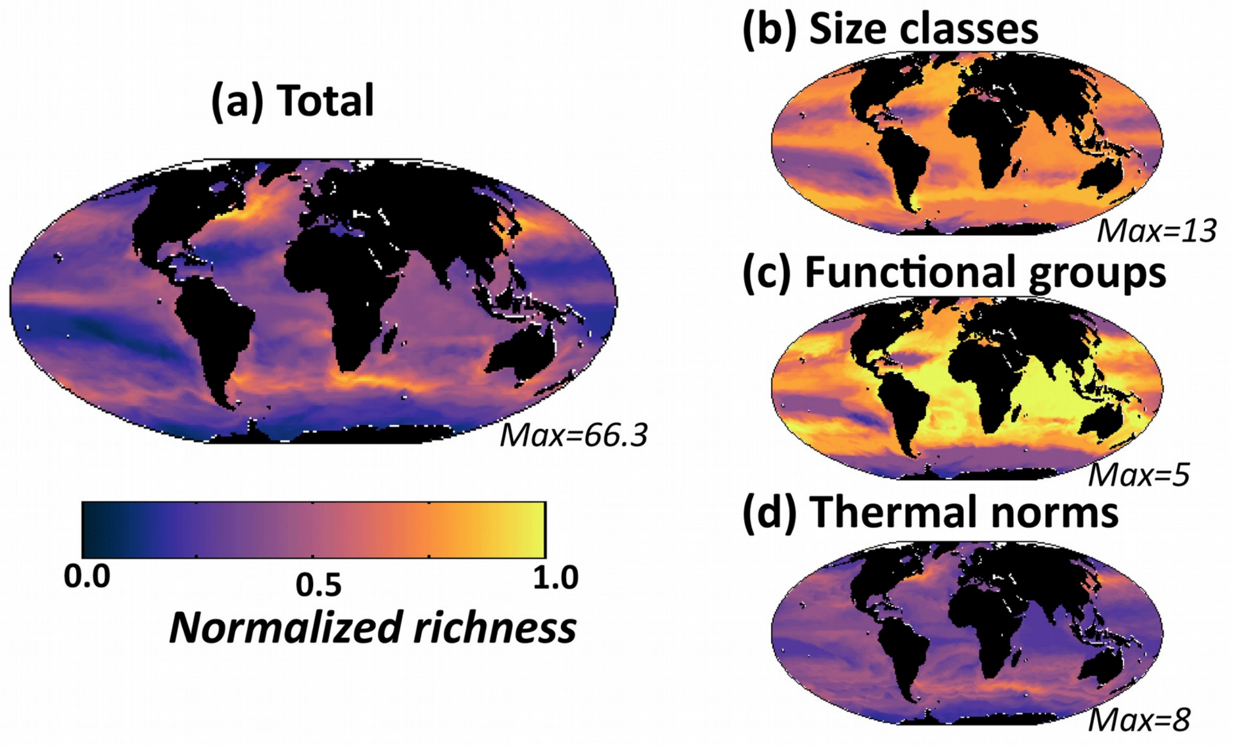


Xu et al. (2021)

Most current models mix both approaches

- The different modeling approaches are not hermetically separated
- Most models mix to some extent PFT and trait-based modeling formalisms





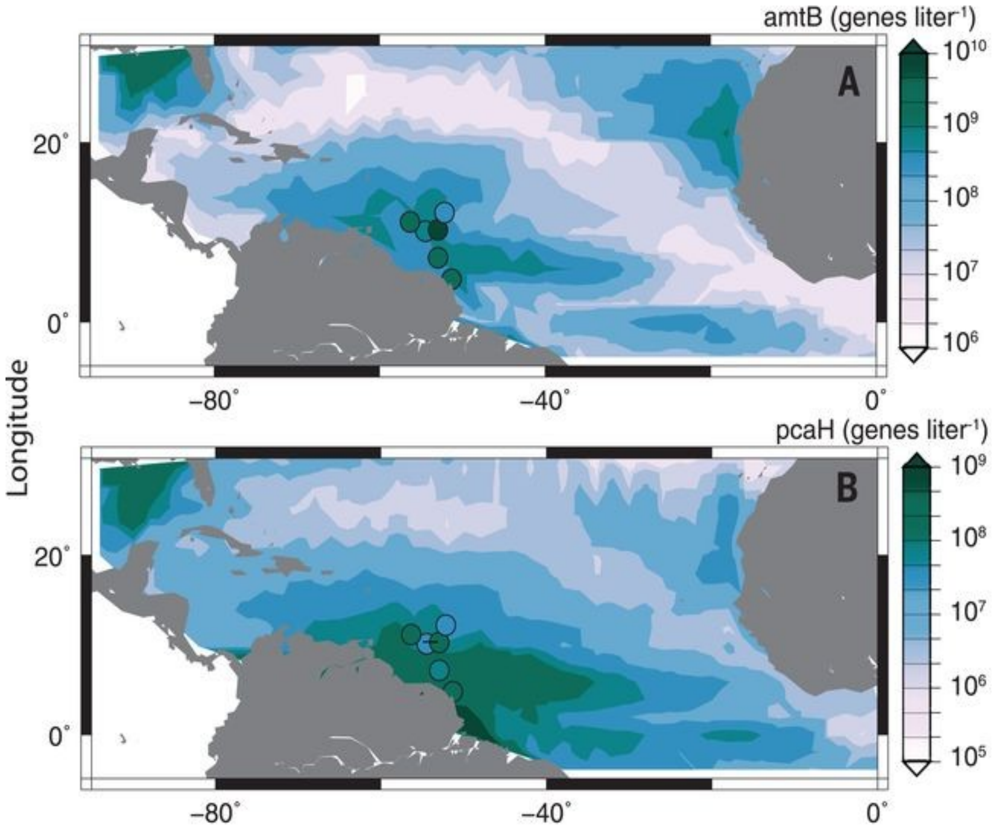
A version of the DARWIN model (Dutkiewicz et al., 2020)

Gene-centric models

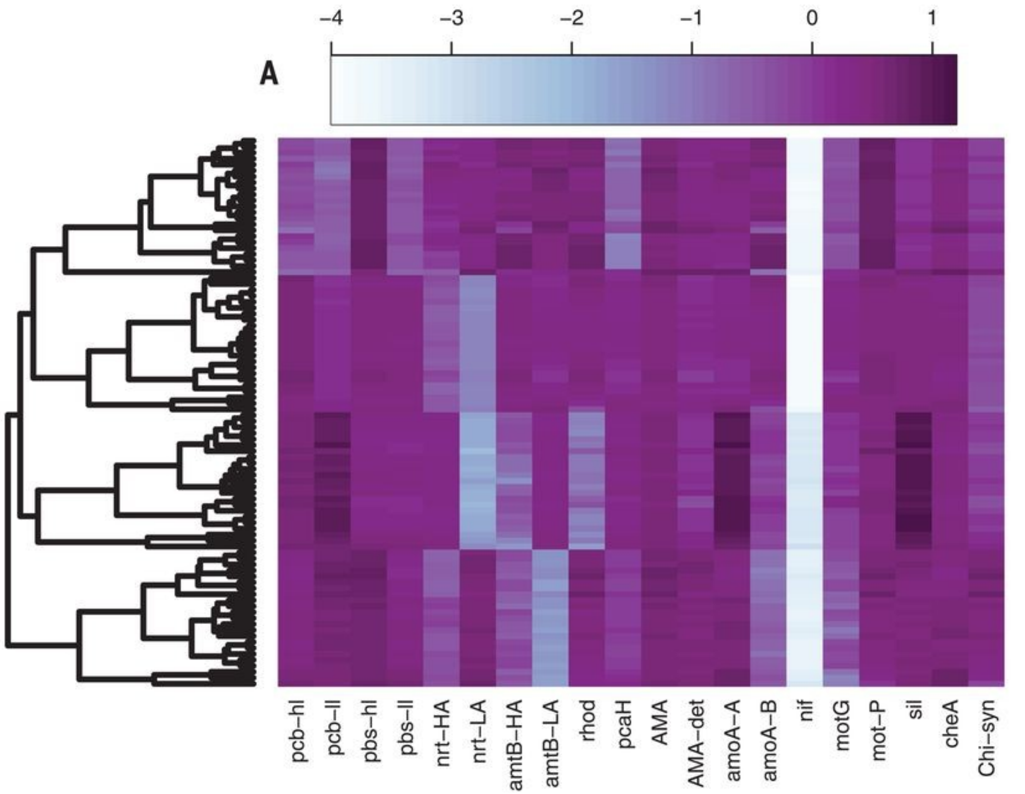
- Bringing together (meta)genomic data and biogeochemical models is challenging
- A major difficulty is that they differ in the considered currency: ‘omics data refer to genomes, proteins and metabolites; biogeochemical models refer to concentrations, biomass and biogeochemical functions
- A functional gene-centric approach: organisms are grouped according to their functional genes/metabolisms (Reed et al., 2014)
- As most organisms in the sea are uncultured, simulating their genes is impossible. An alternative is to randomly allocate genes from a know pool to construct a set of organisms (Cole et al., 2017). And the environment selects.

GENOME model

- A example of a gene-centric modeling study in the Atlantic Ocean (Cole et al., 2017)



Surface genes concentration in June



Metagenomes in the Amazon river plume in June clustered by similarities

- These approaches linking omics and biogeochemical/ecosystem are still in their infancy but are rapidly growing

Final words

- A brief and subjective overview of biogeochemical/ecosystem modeling
- Many aspects have been omitted: upper trophic levels, evolution, niche-modeling, micro-nutrients, diagenetic/benthic, ...
- Many challenges have not been mentioned (and I certainly do not know all of them)
- One of these (not clearly stated) challenges is to bring together an increasing number of very diverse expertise: mathematics, computer science, physics, physiology, biogeochemistry, ecology, ‘omics, …
- Models are not the real world. They are always imperfect and necessarily show some level of deficiency