The Climate Ocean and Sea Ice Model (COSIM) project
Computational and Theoretical Science Divisions

Trace Gas Emissions from POP

Scott Elliott and Mathew Maltrud

Collaborators: LLNL, NCAR, PNL, ANL, ORNL, WHOI, The CODiM Group (International S modelers)

Sponsors: DOE Scientific Discovery through Advanced Computing (SCIDAC), Climate Change Prediction Program (CCPP), NSF, SOLAS

MAJOR POINTS

- Motivation -dynamic marine emissions fields for CAM/CCSM
- Modular trace gas geocycling driven by or ported to DML
- Maintains POP performance, portability and transparency
- About one dozen volatile source compounds tested or developed
- Oceanic reduced sulfur now dynamic and coupled to CAM/CCSM
- Provide background, demos, case studies and discuss future
- Draw on Najjar, PMEL, ZZZ and others including Julia

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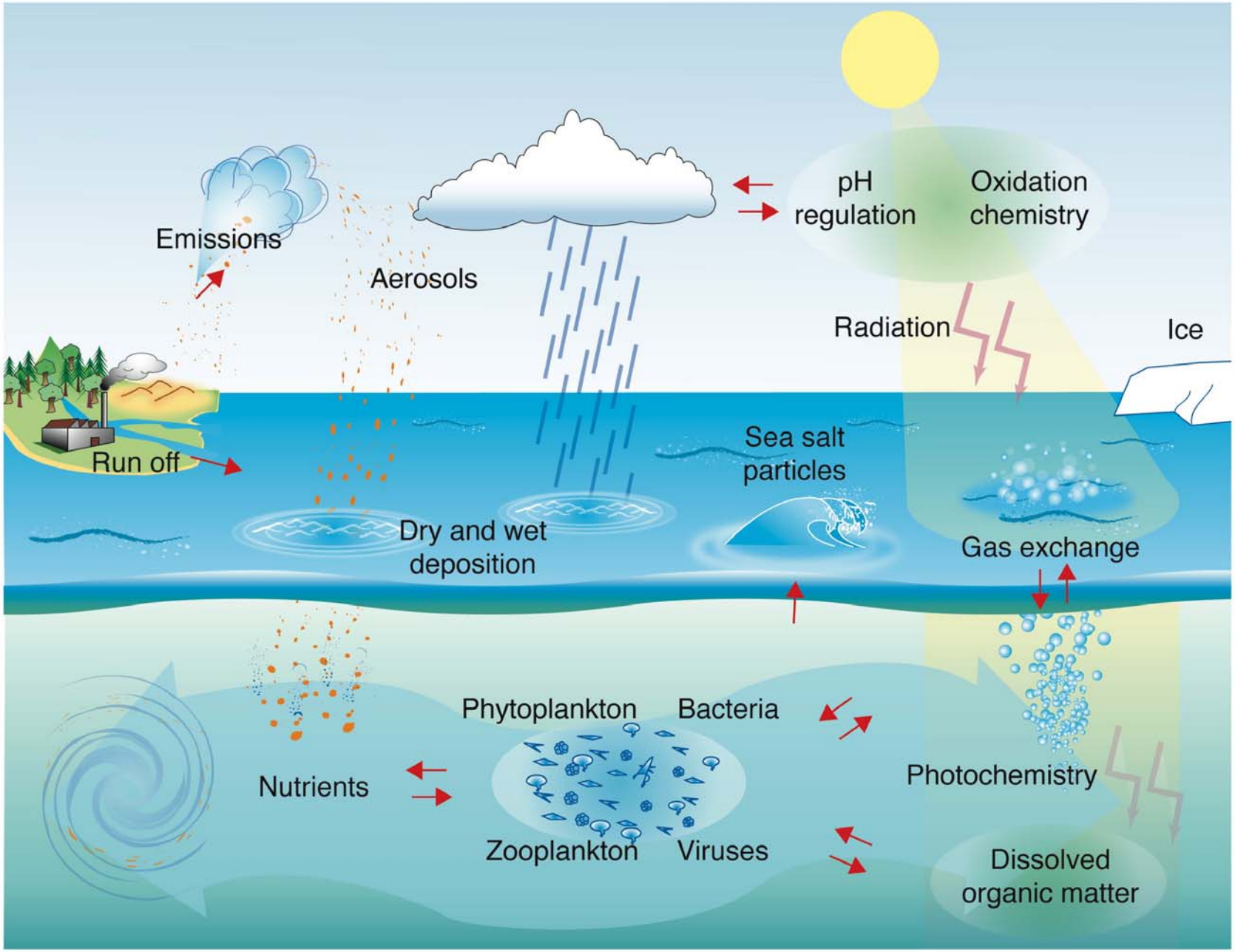
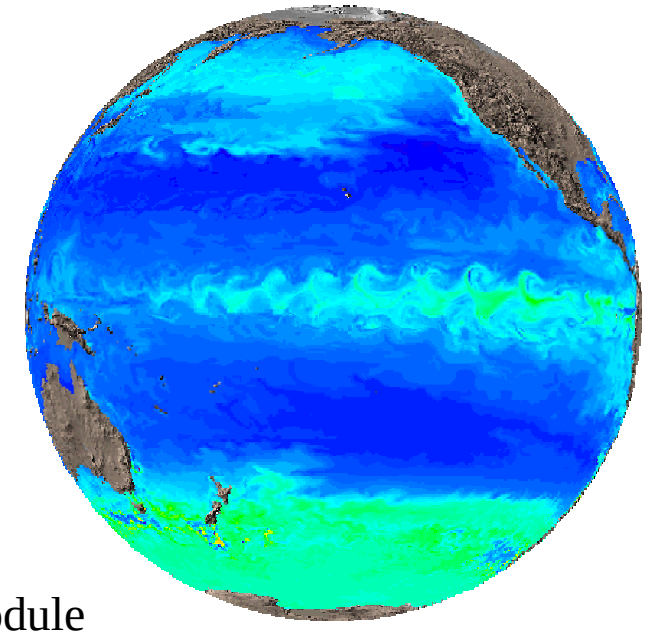
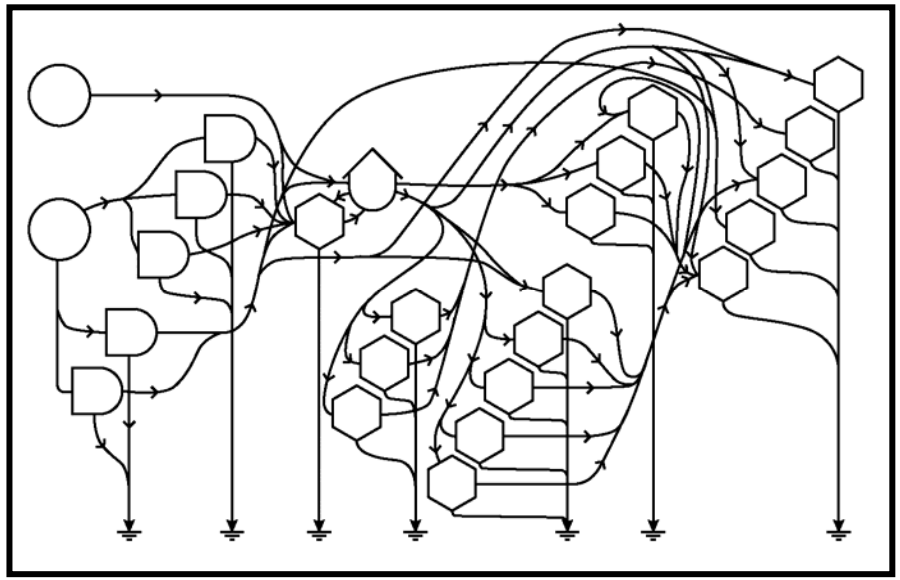

pH
regulation
Oxidation
chemistry
Emissions
Aerosols
Radiation
Ice
Run off
Sea salt
particles
Dry and wet
deposition
Gas exchange
Phytoplankton
Bacteria
Nutrients
Photochemistry
Zooplankton
Viruses
Dissolved
organic matter

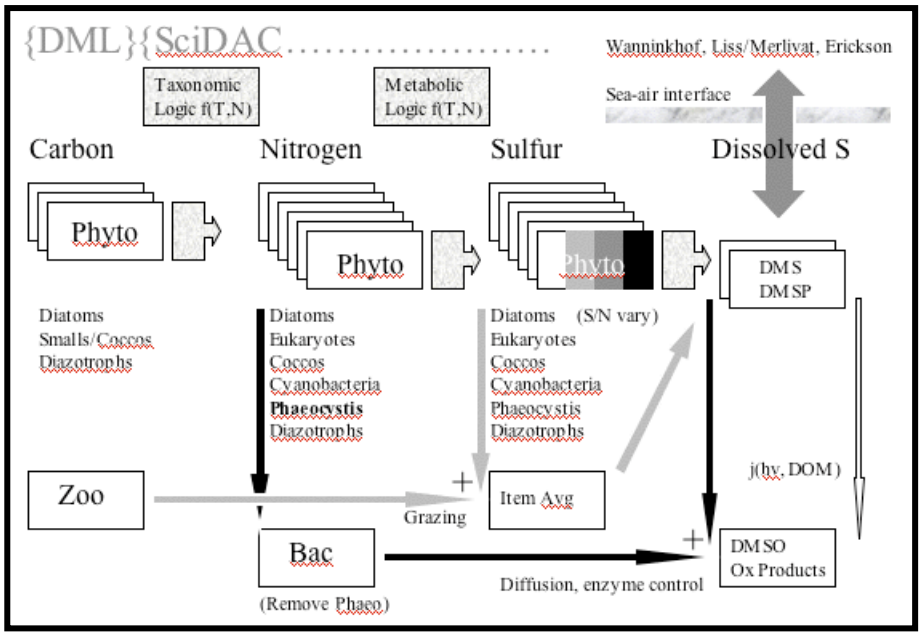
OGCM



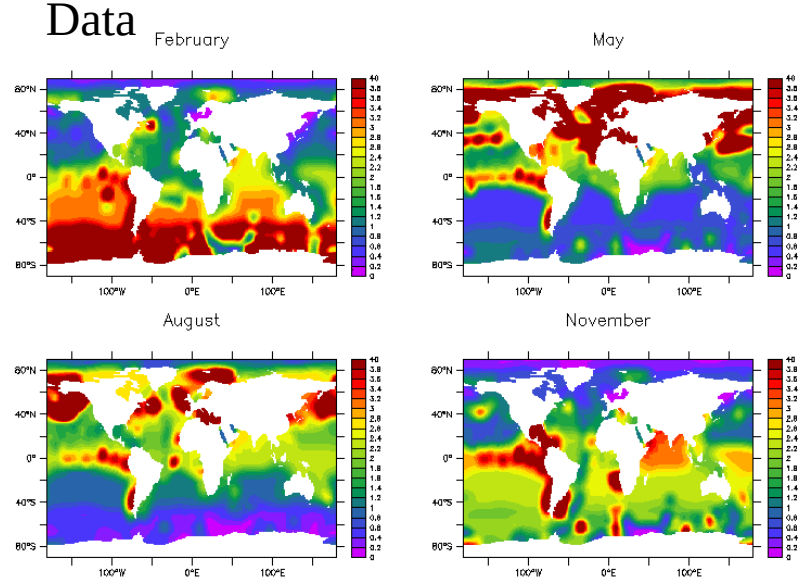
Ecodynamics

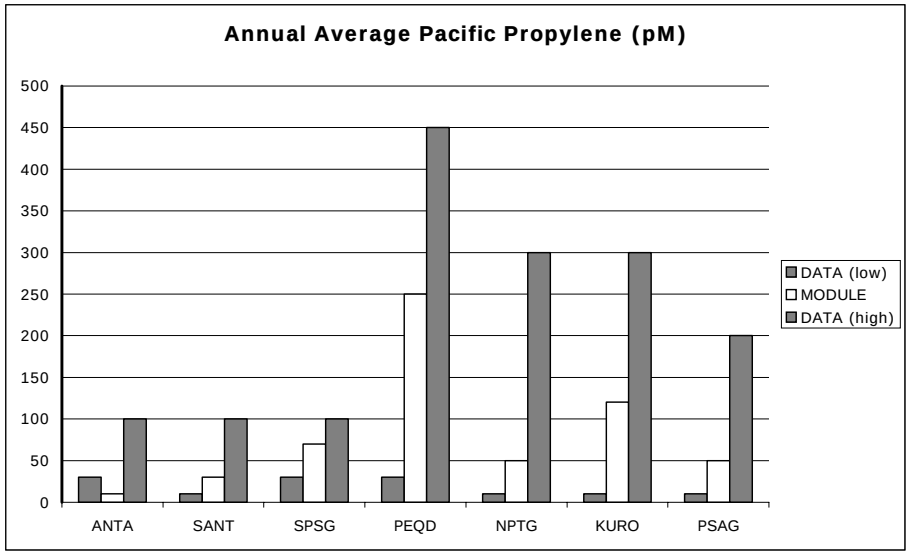


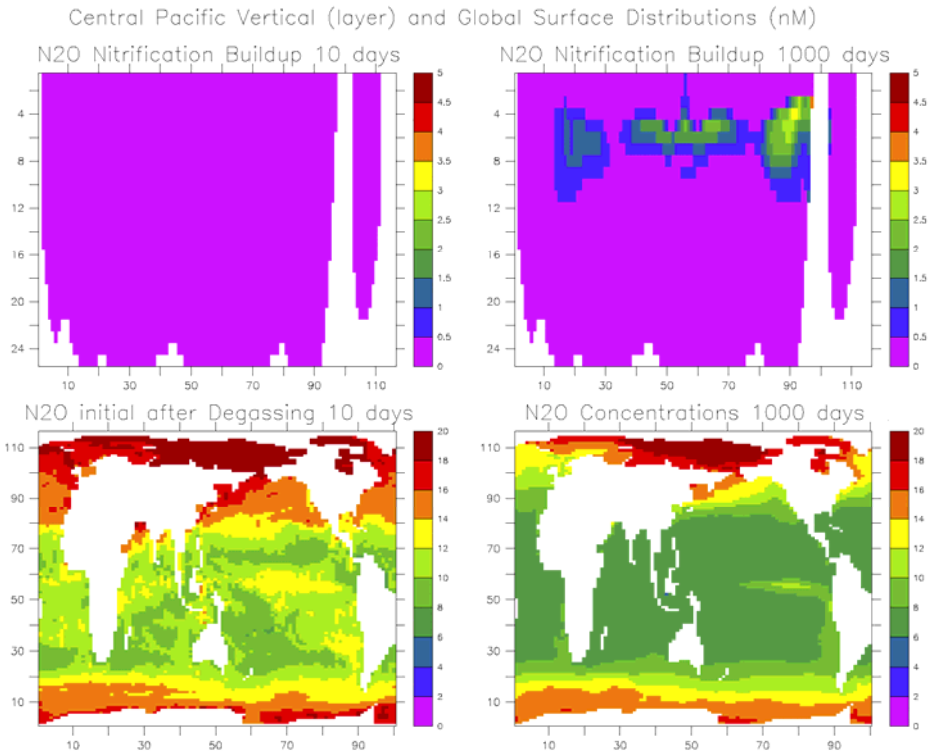
Sulfur module



Data







MECHANISMS SO FAR

- Demonstrations
  - -Methyl Halides
  - -Propylene
  - -Nitrous Oxide
  - -Methane
  - -Ammonia
- Published
  - -Carbon Monoxide
  - -Dimethyl Sulfide
  - -Collective Methods
- In Prep -Carbonyl Sulfide

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Effects of marine photochemistry

Element cyling

C, S, P, N, trace metals (Fe,Mn)

CDOM + UV light

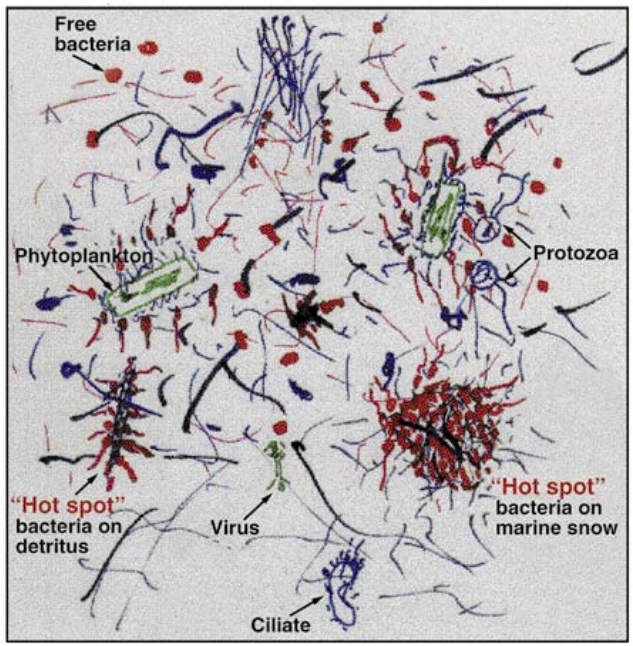
Biota

Prod. of labile C, nutrients, radicals

Water transparency

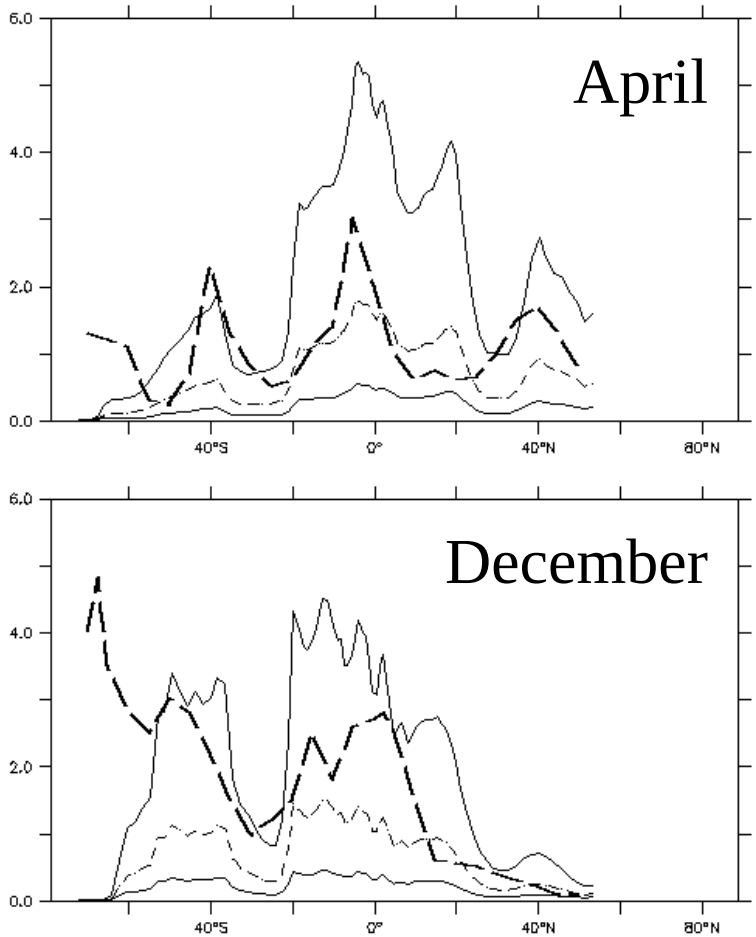
Photobleaching

Fichot, 2006
Azam 1998



Carbon Monoxide

- **PMEL cruises at 140W**
- **POP with sensitivity test quantum yield**

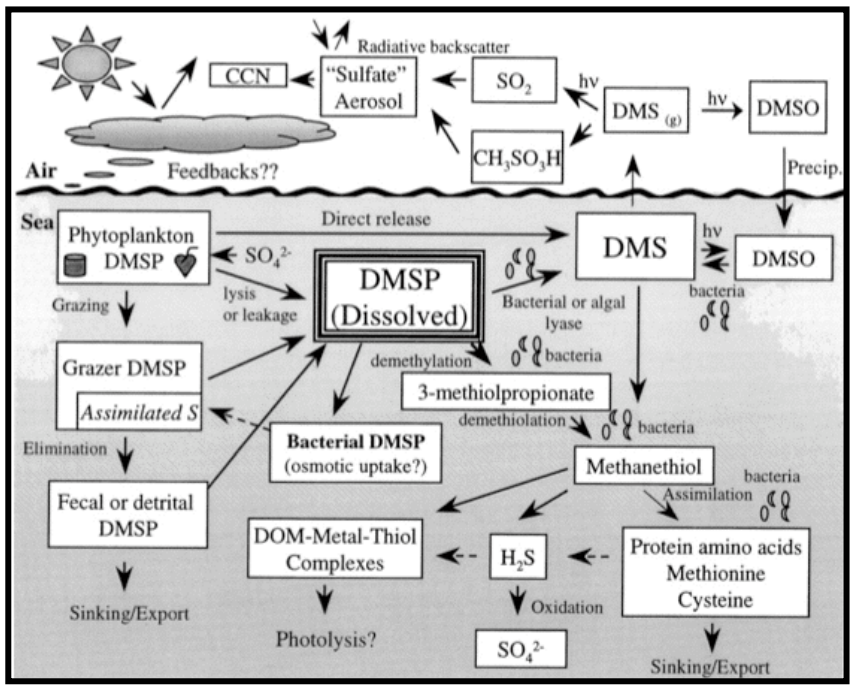


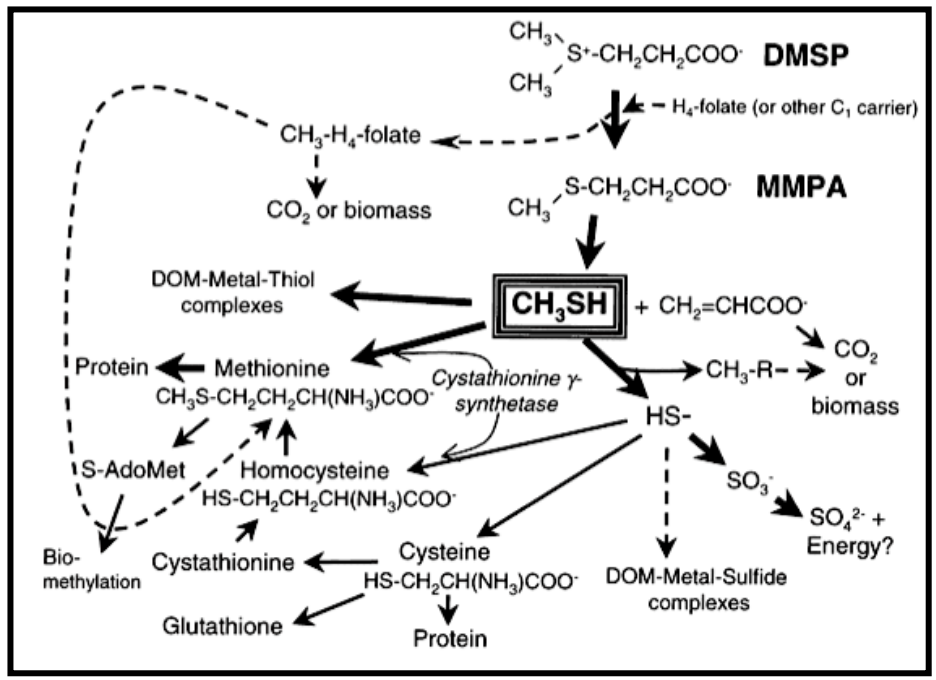
DMS BIOGEOCHEMISTRY

- Stresses upregulate about a dozen close organic relatives
- Transformation in the column
- Yield and loss also complex, set by microbial metabolics

Table 1 Computed *in vitro* half-lives for •OH radical

Compound	Concentration ($mmol\,l^{-1}$)	Rate constant* ($M^{-1}\,s^{-1}$)
DMSP	150–450†	3×10^{8}
Acrylate	~1–40?	5.6×10^{9}
DMS	~1–40?	1.9×10^{10}
DMSO	30–90†	6.6×10^{9}
MSNA	?	9×10^{9}
Glutathione	2.4‡	1.4×10^{10}
Ascorbate	1–6§	1.1×10^{10}



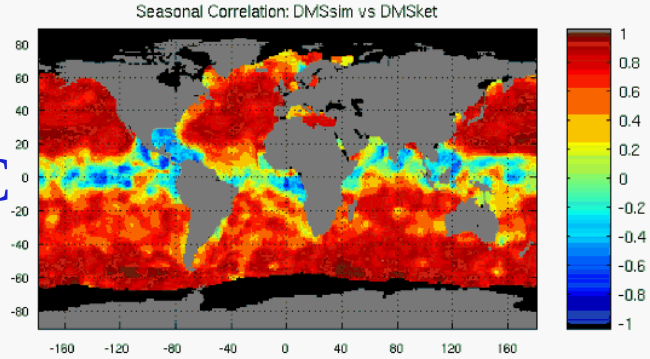


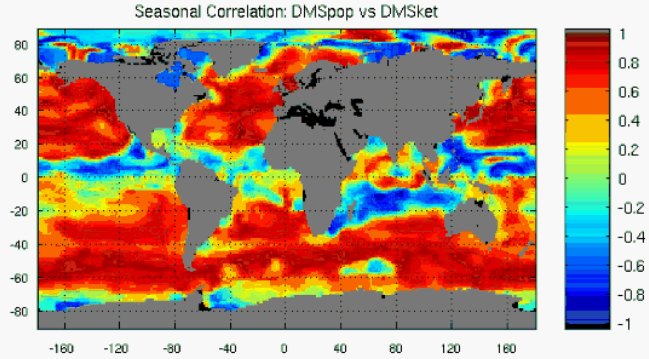
DMSmodel vs DMSkettle

Statistical

Dynamic

BARC





LANL

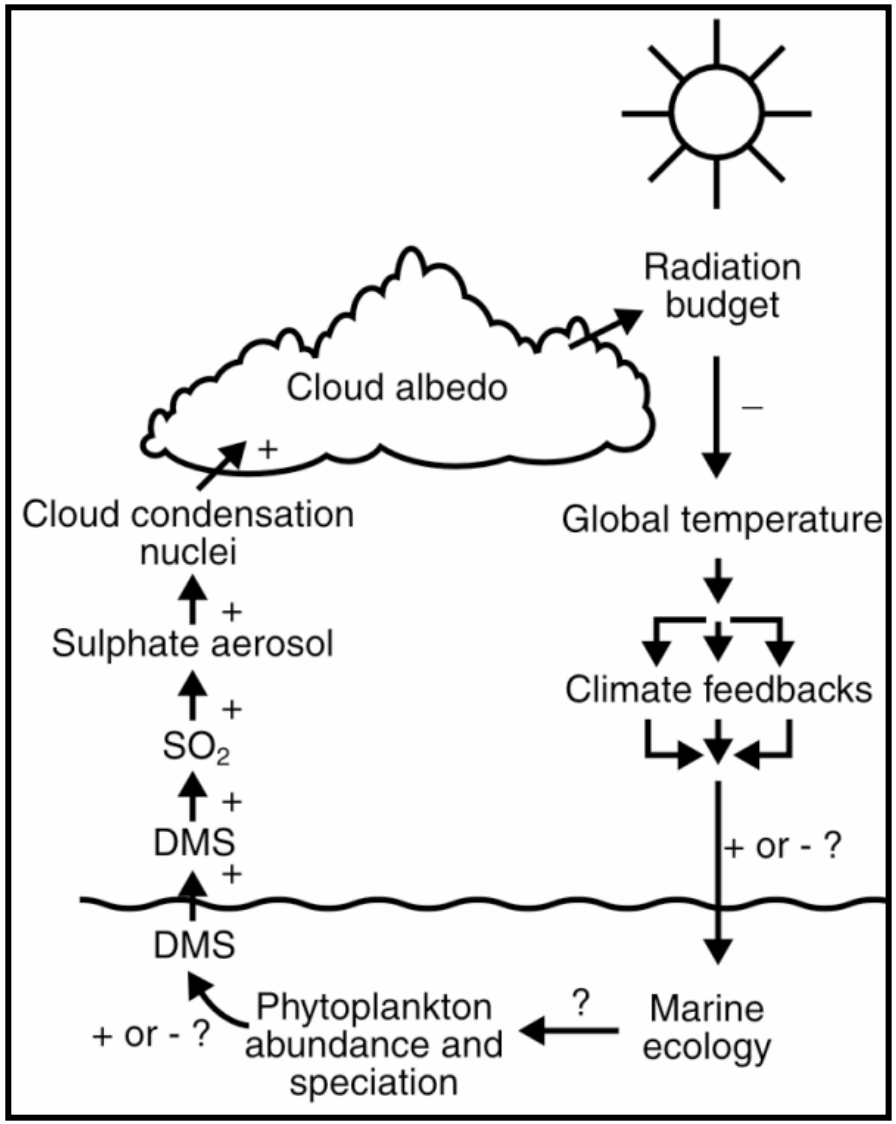
PAR

NOR

HAD

HAM

CLAW PROJECT



- Community driver continues to be CLAW
- Magnitude, sign of ecosystem effects remain uncertain
- Only detailed modeling can alleviate the situation
- That's SciDAC working with CCSM
- LLNL, NCAR, PNL, ANL, DML all in coupling experiments

Charlson et al. 1987

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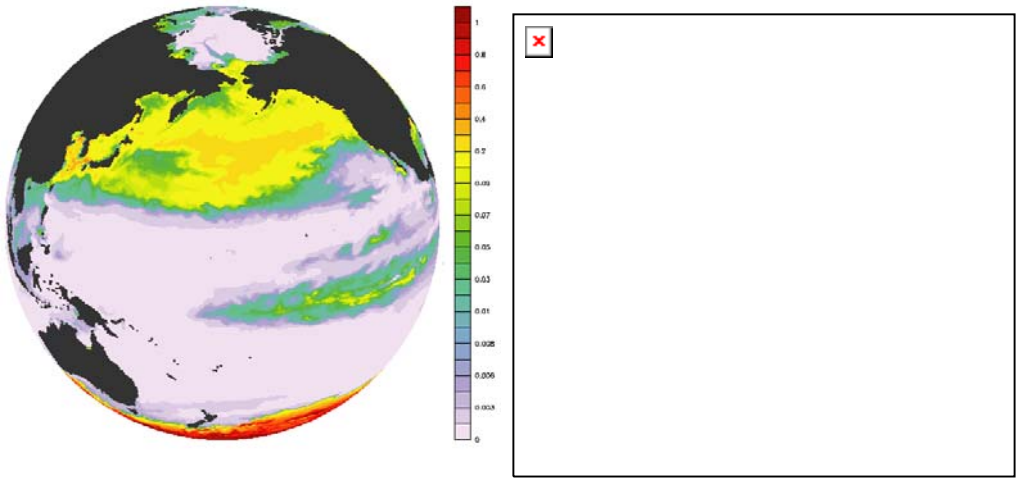
NH_4^+ μM

NH_3 pM



November 1995

Classic of the month

A Relational Model of Data for Large Shared Data Banks

E. F. Codd

Reprinted from *Communications of the ACM*, Vol. 13, No. 6, June 1970, pp. 377-387. Copyright Association for Computing Machinery, Inc.

FUTURE WORK

- Piston velocity issues
- Collective NMHC and the ozone system
- Ammonia as ocean acidifies
- Unified multiclass bacteria
- Also move beyond gases
- Organics at interfaces
- Fe/N/S(/Fe/N…) coupling
- RDB and CASE coding

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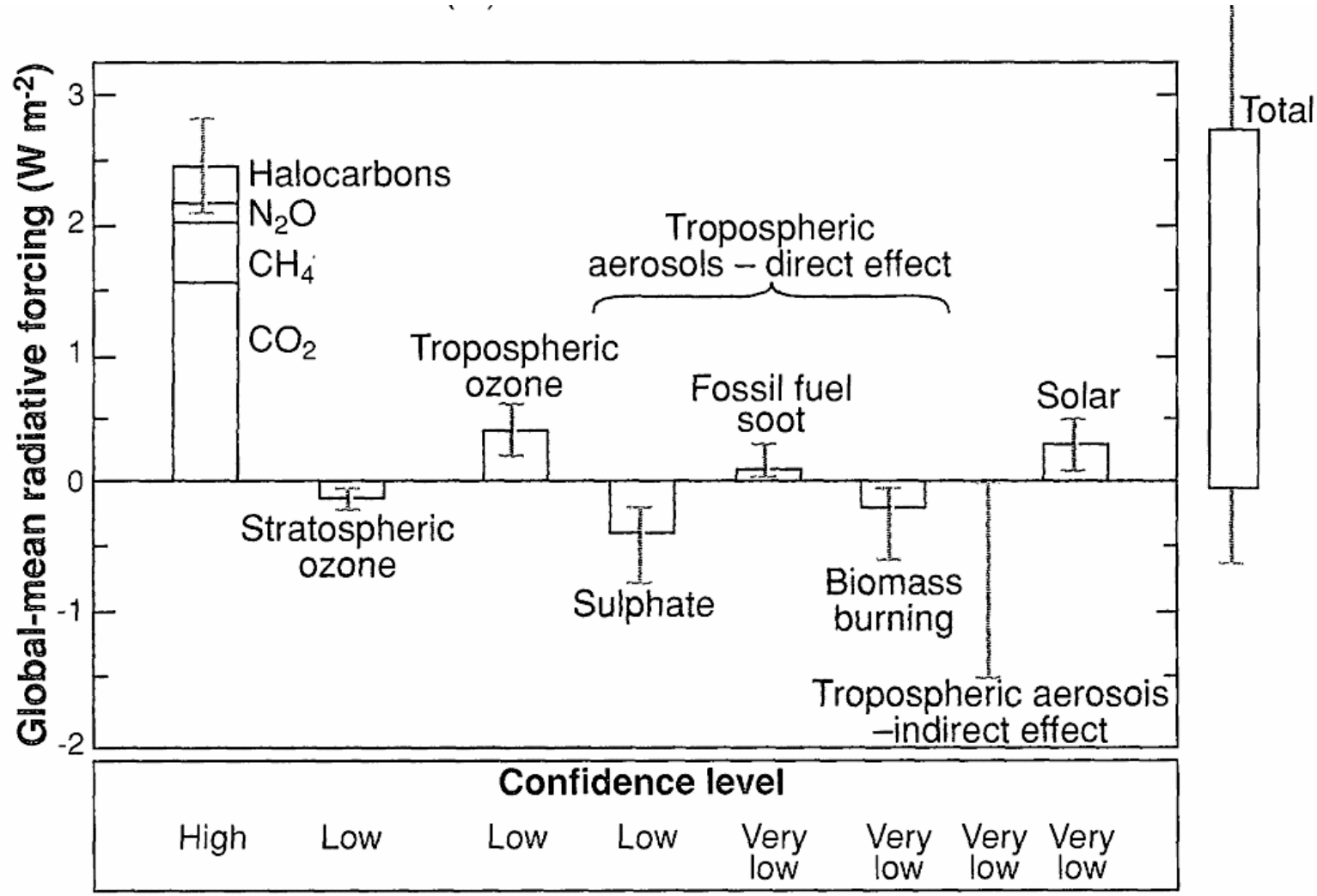
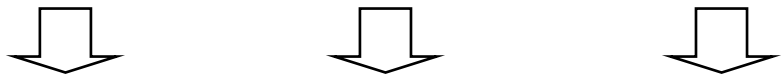
EXTRAS

Schwartz-Andreae Histogram



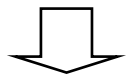
Teleconnection Strategy

Element	**C**	**N**	**S**	**Fe**
Primary form	Carbonate	NO_3^-	SO_4^-	Fe^{2+}
Rank	CO	NH_3/NH_4^+	DMS(P,thiol)	Dust
	NMHC	GBT	S metabolism	Coatings
	DOM, CDOM	N_2O	OCS, MTC	Complexes
	Surfactants	DON	H_2S	C ligands
	CH_4		Complexes	Fe^{3+}



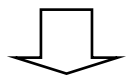
Eco/geo unity

Taxonomy, bacteria



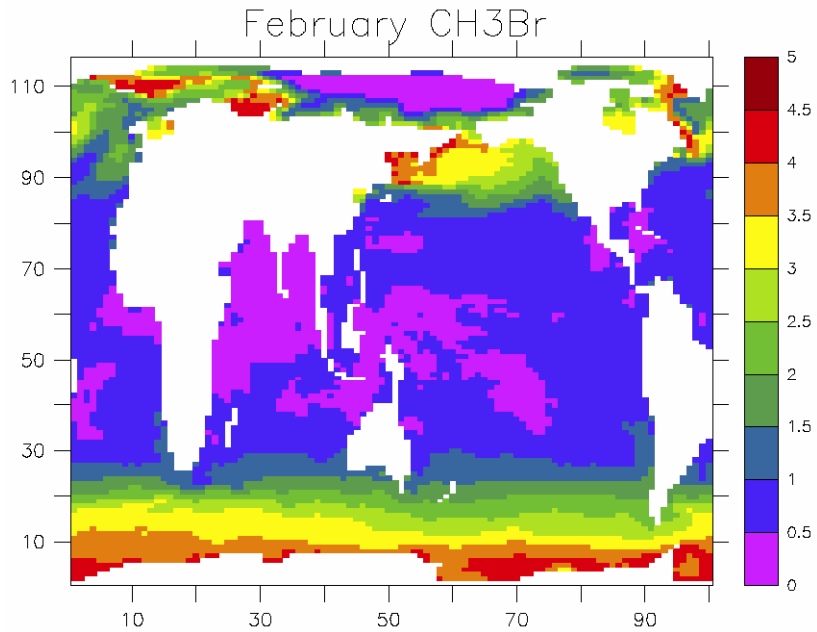
Ice and shelf domains

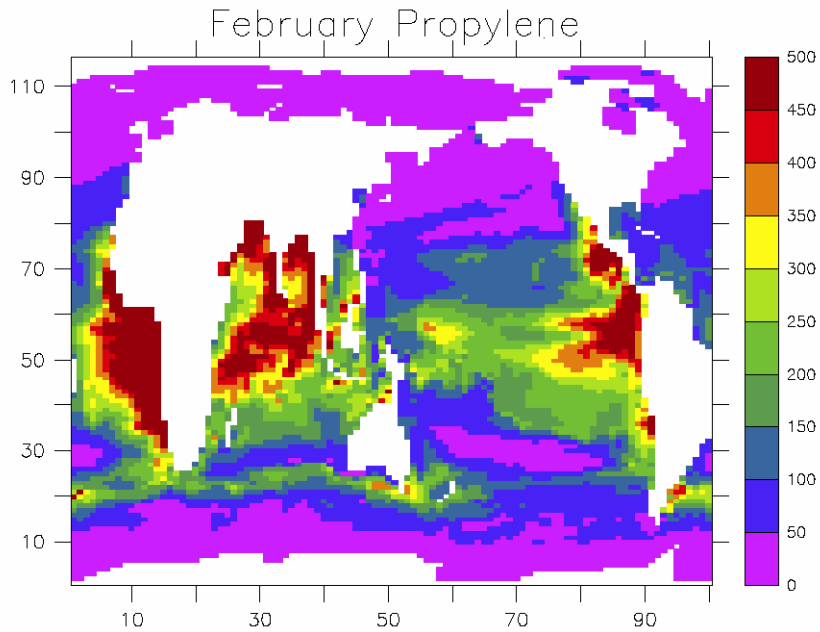
Systems model

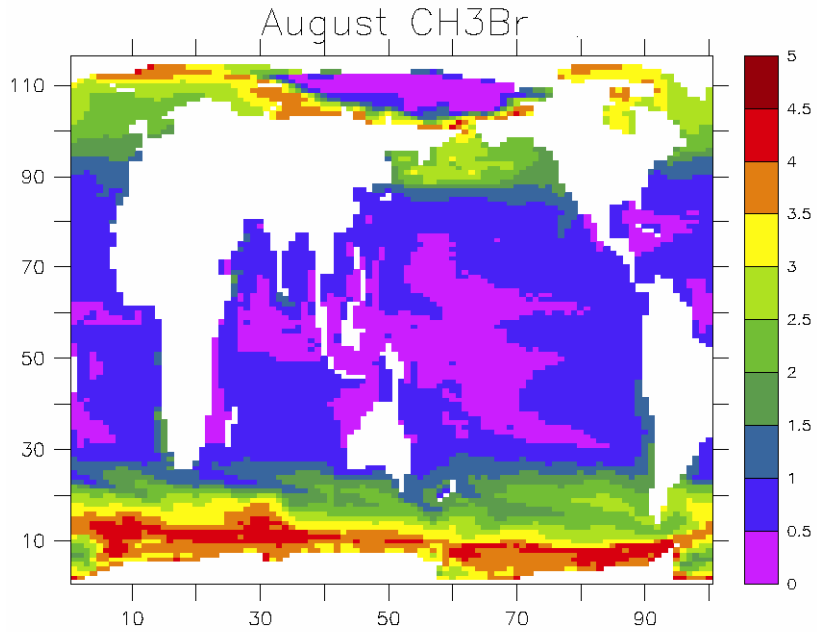


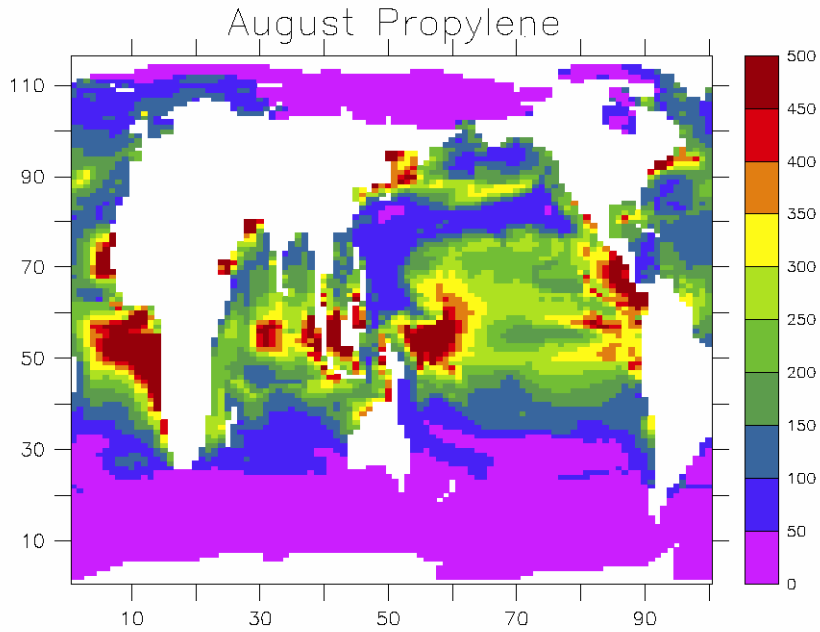
Planetary scale engineering

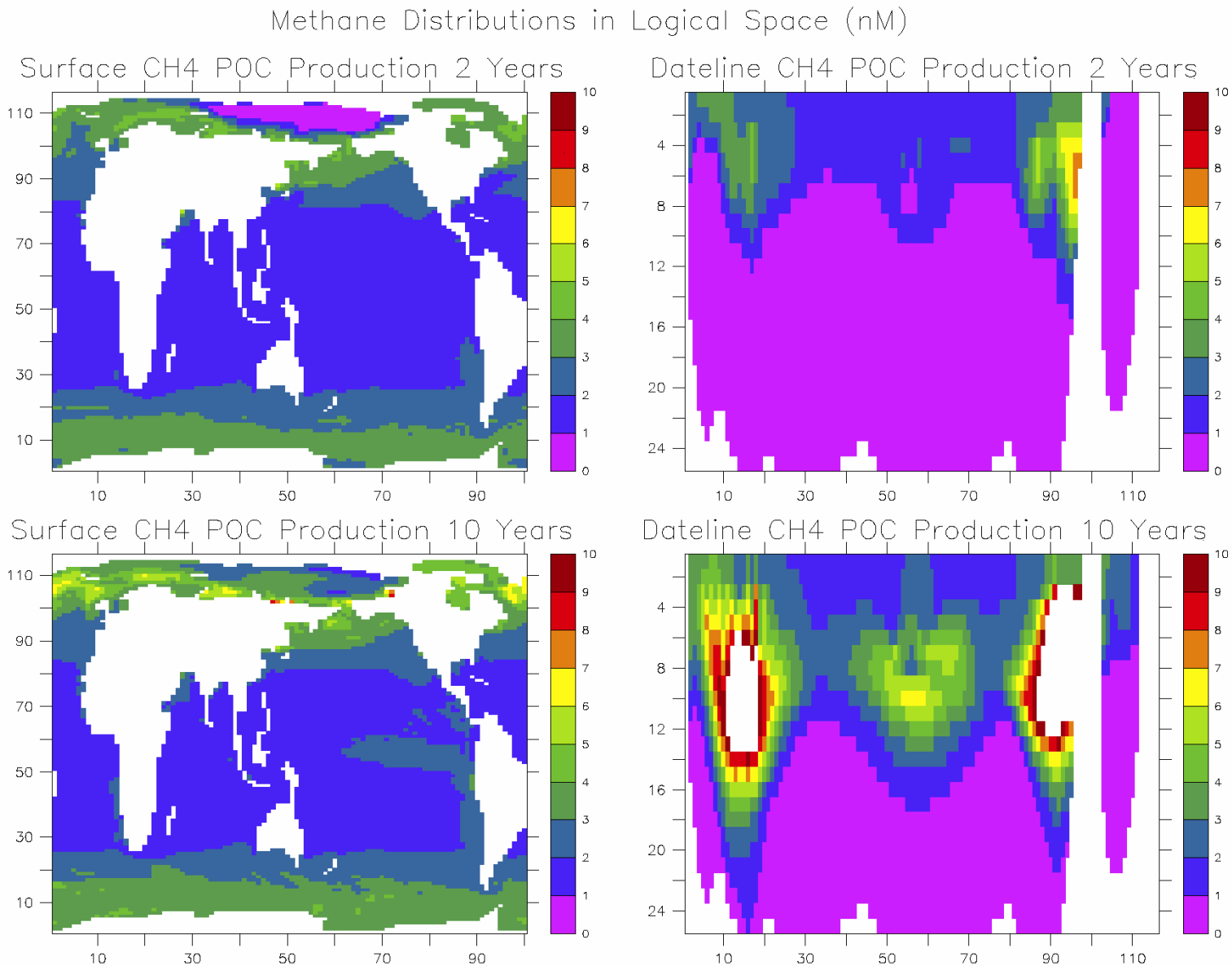
Selected Monthly Average Surface Distributions (pM)



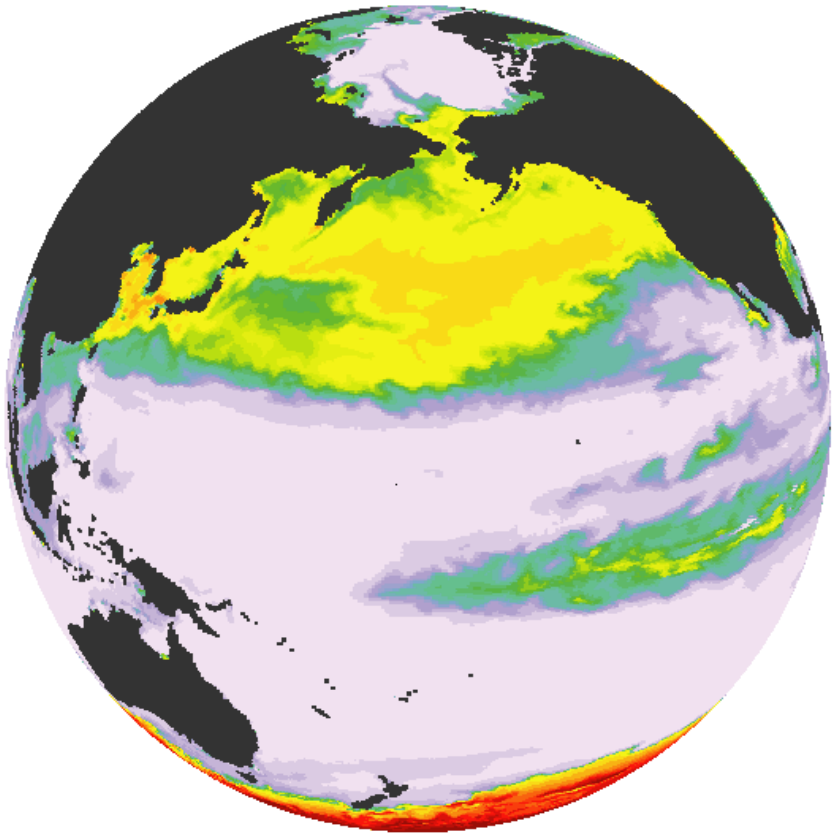




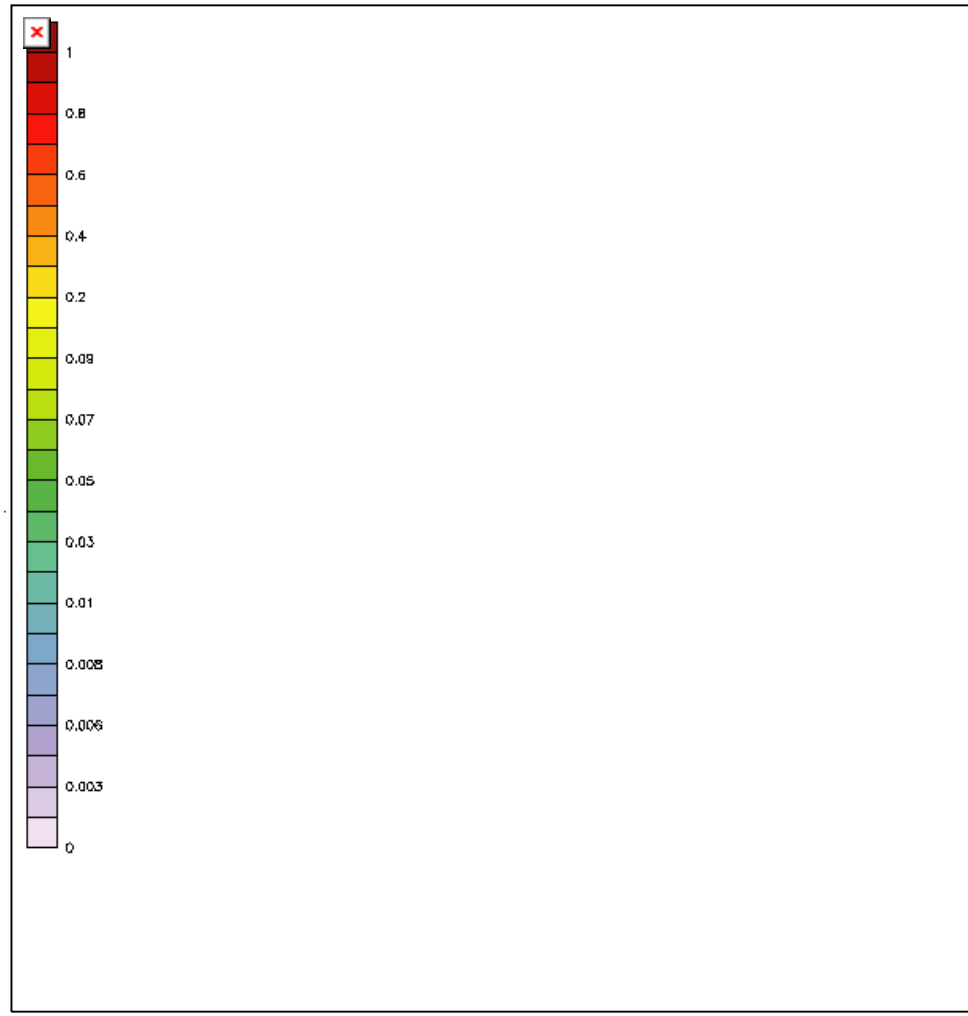



Methane Distributions in Logical Space (nM)
Surface CH4 POC Production 2 Years
Dateline CH4 POC Production 2 Years
Surface CH4 POC Production 10 Years
Dateline CH4 POC Production 10 Years
10
30
50
70
90
110
4
8
12
16
20
24
0
1
2
3
4
5
6
7
8
9
10

NH_4^+ Seawater μM



NH_3 Boundary Layer pM



Gunson Temperatures

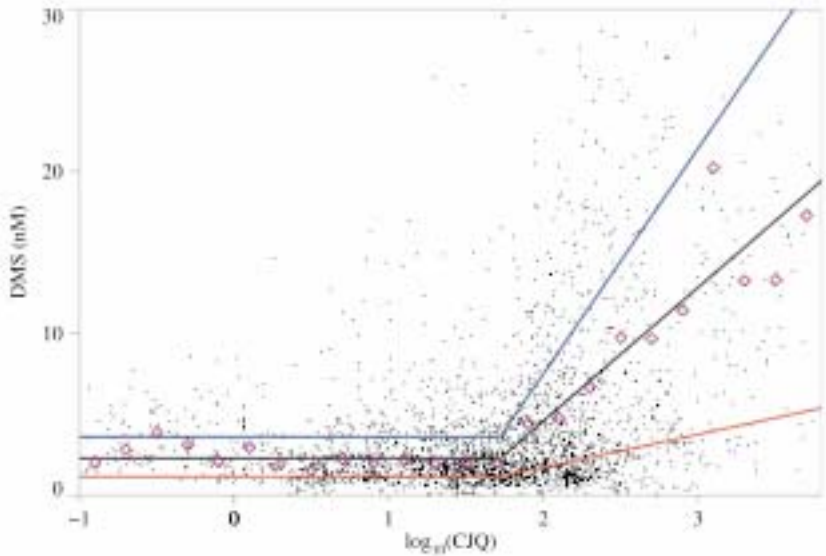


Figure 1. Ocean surface DMS vs. $\log_{10}$(CJQ): points are raw data from *Kettle et al.* [1999] database, purple diamonds show median (for $\log_{10}(CJQ) < 1.72$) and mean (for $\log_{10}(CJQ) > 1.72$) values over binned data, black line is broken-stick line of best fit to diamond points, blue and red lines are broken-stick lines of best fit to upper and lower fifty percentiles of data points, respectively.

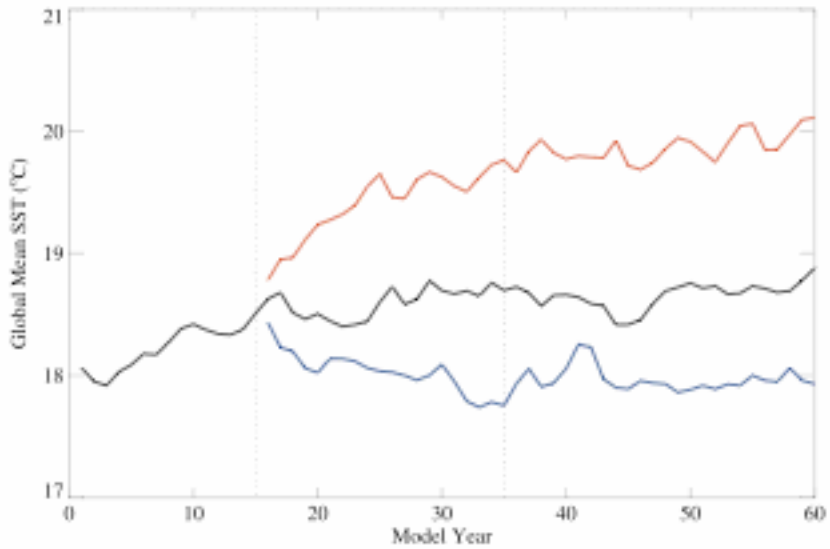
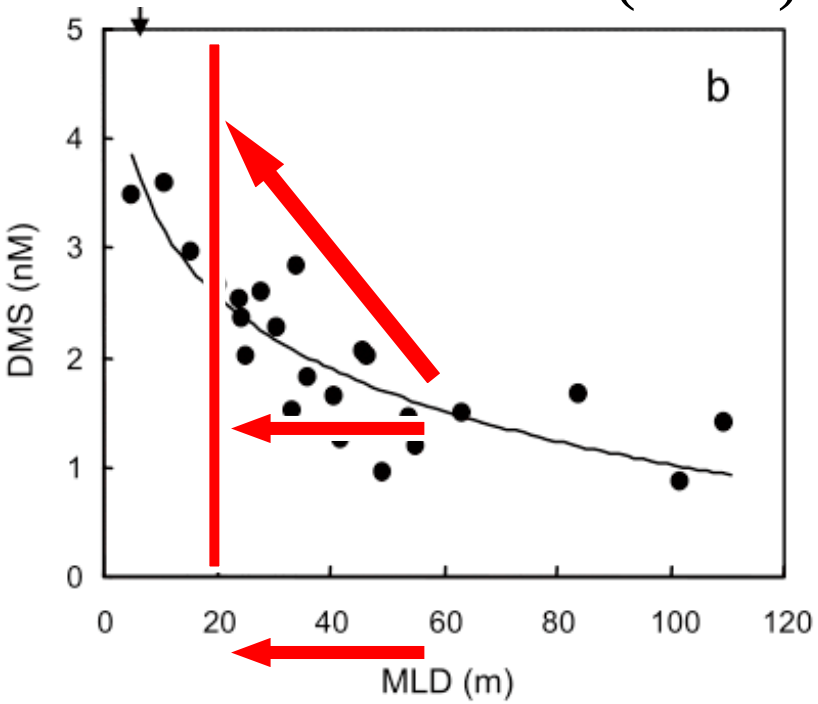
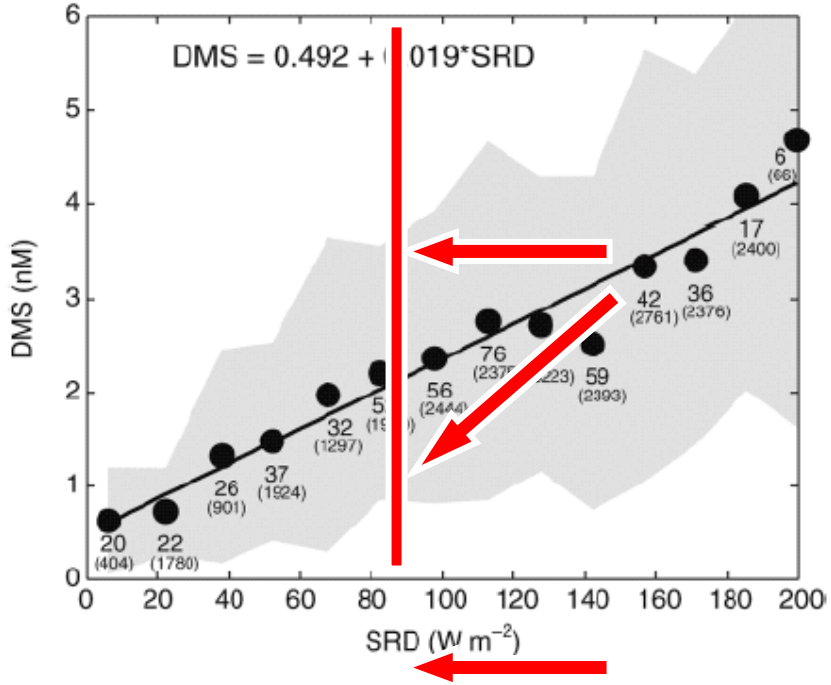


Figure 2. Global Mean SST over the course of the experiment for the control simulation (black), the positive DMS perturbation simulation (blue) and the negative DMS perturbation simulation (red).

Simo group late 90's
Global relation to ln(MLD)



Simo group 2007
Global relation with Dose



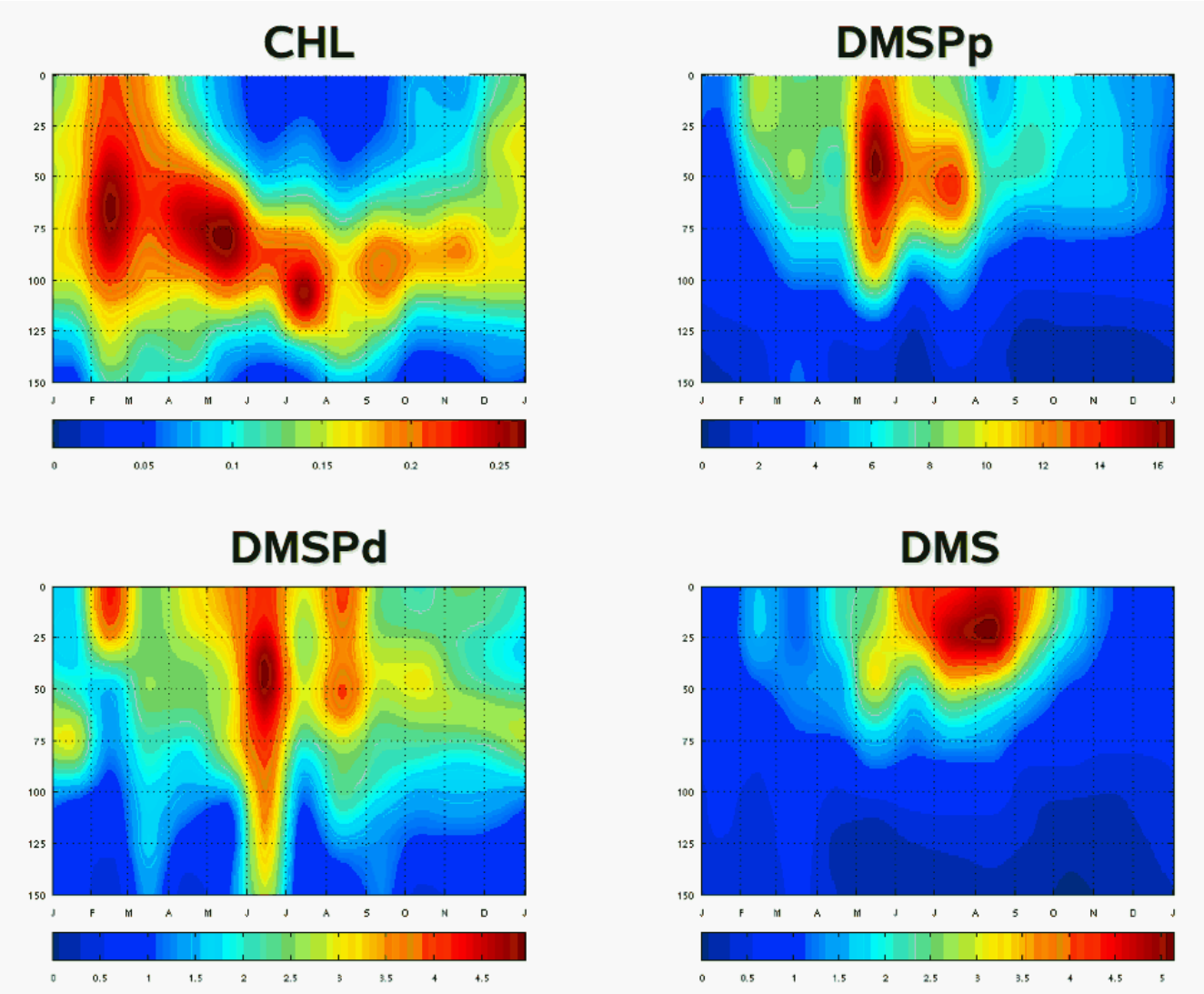
Rafel has proposed the two best correlations but they are very closely related, and the planet will not simply slide along his relationships. Imagine moving systems into the anthropocene. We can readily shift individual ecologies independently to new curves, e.g.

MLD case - Shoaling could favor small producers over large areas while also increasing their stress levels, or else lead to a prokaryote dominance.

SRD case - Cloud cover could add nutrients for eukaryotes, or cut UV thus lowering stress and increasing bacterial demand/consumption.

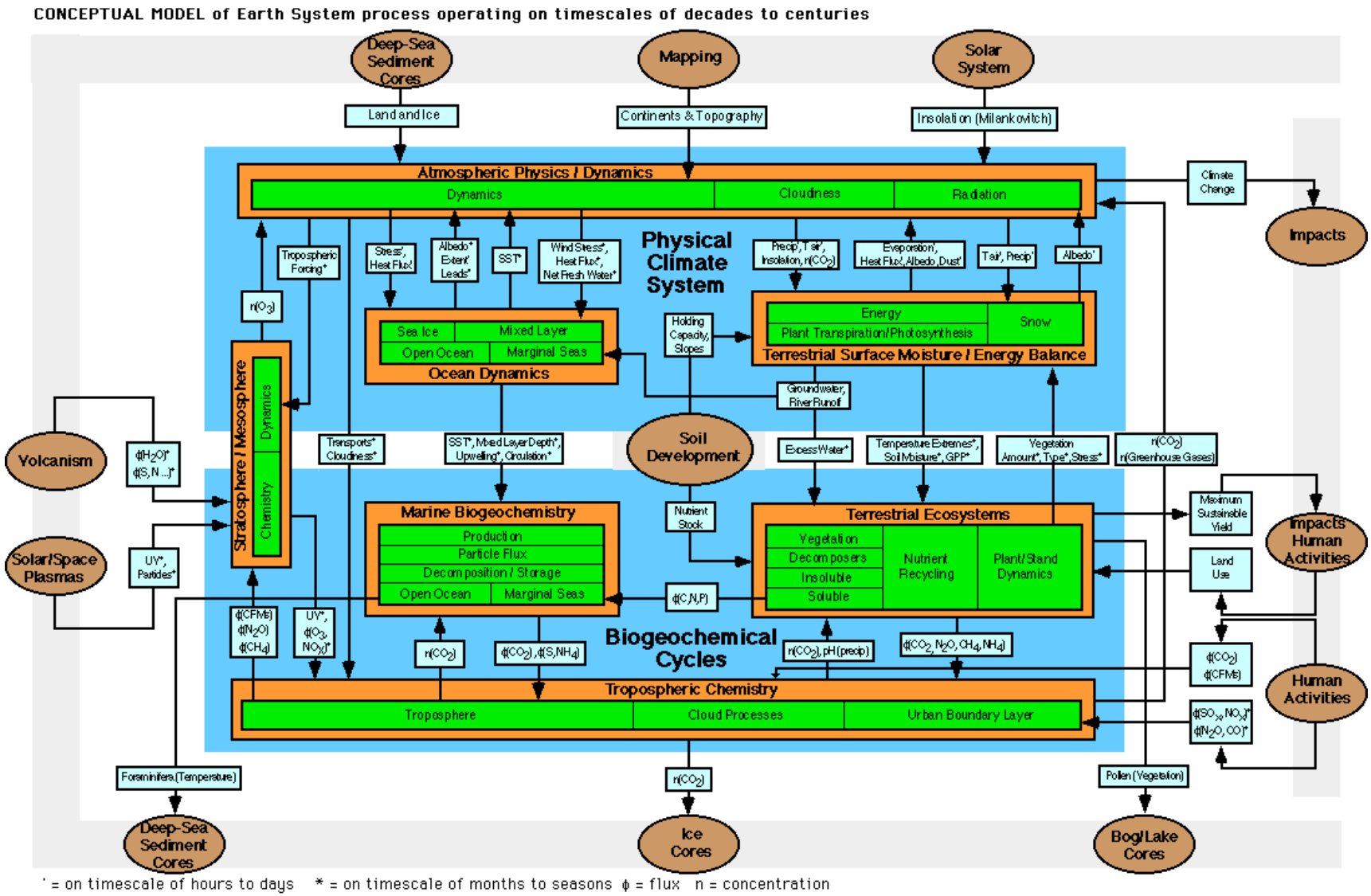
There is thus no escaping the need for detailed biogeographical integrations.

Sargasso Sulfur Climatology



BATS data and Vallina Thesis 2007

The Bretherton Horrendogram



Mitchell K. Hobish, Earth Systems Science, Section 16, Remote Sensing Tutorial
http://rst.gsfc.nasa.gov/Sect16/Sect16_3.html