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

Biogeochemistry in Los Alamos COSIM: High Latitudes Processes

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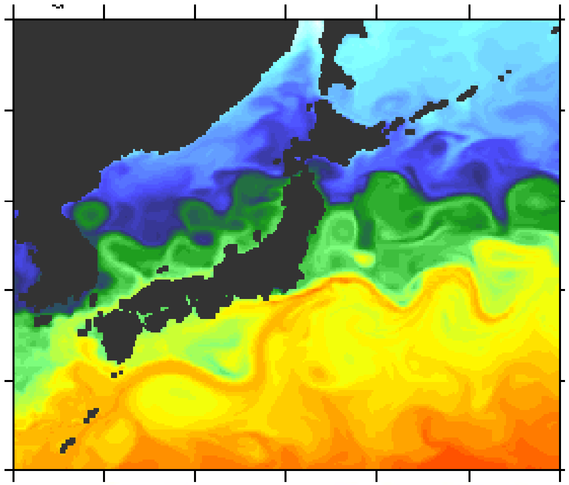
Collaborators:

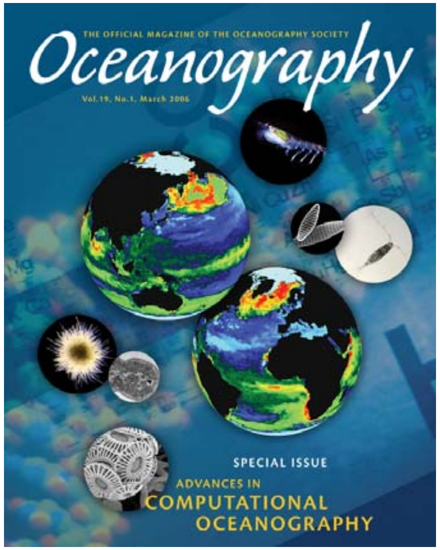
Current: NYU, Stanford, Griffith (Australian Antarctic Division)
Potential: IARC, UTSA, others?

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

TALK OUTLINE

- **A bit of general COSIM background leading to the new emphasis**
- **High latitude deficiencies particularly painfully for biogeochemists**
- **Samples problems: chlorophyll, photochemistry, DMS**
- **So…winterize biogeochemical ocean models beginning from sulfur**
- **Show demonstration of capability for ice algae in CICE**
- **Quarterly maps for the pan-Arctic situation, local time series**
- **New collaborations needed, and planning**





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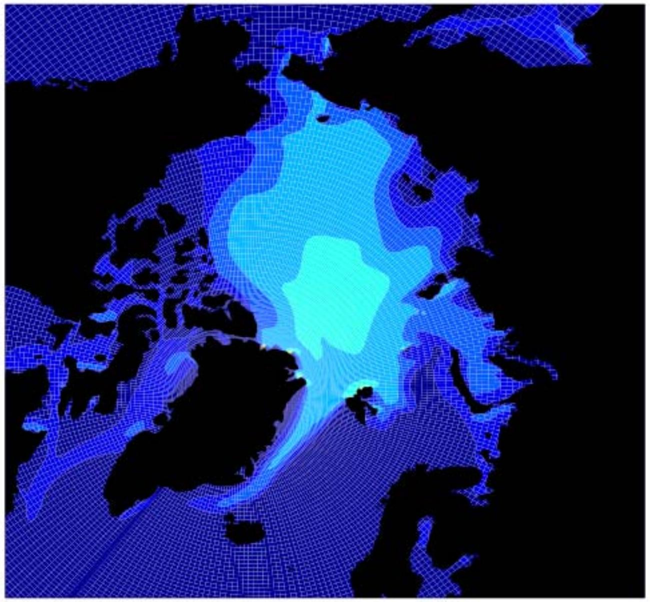
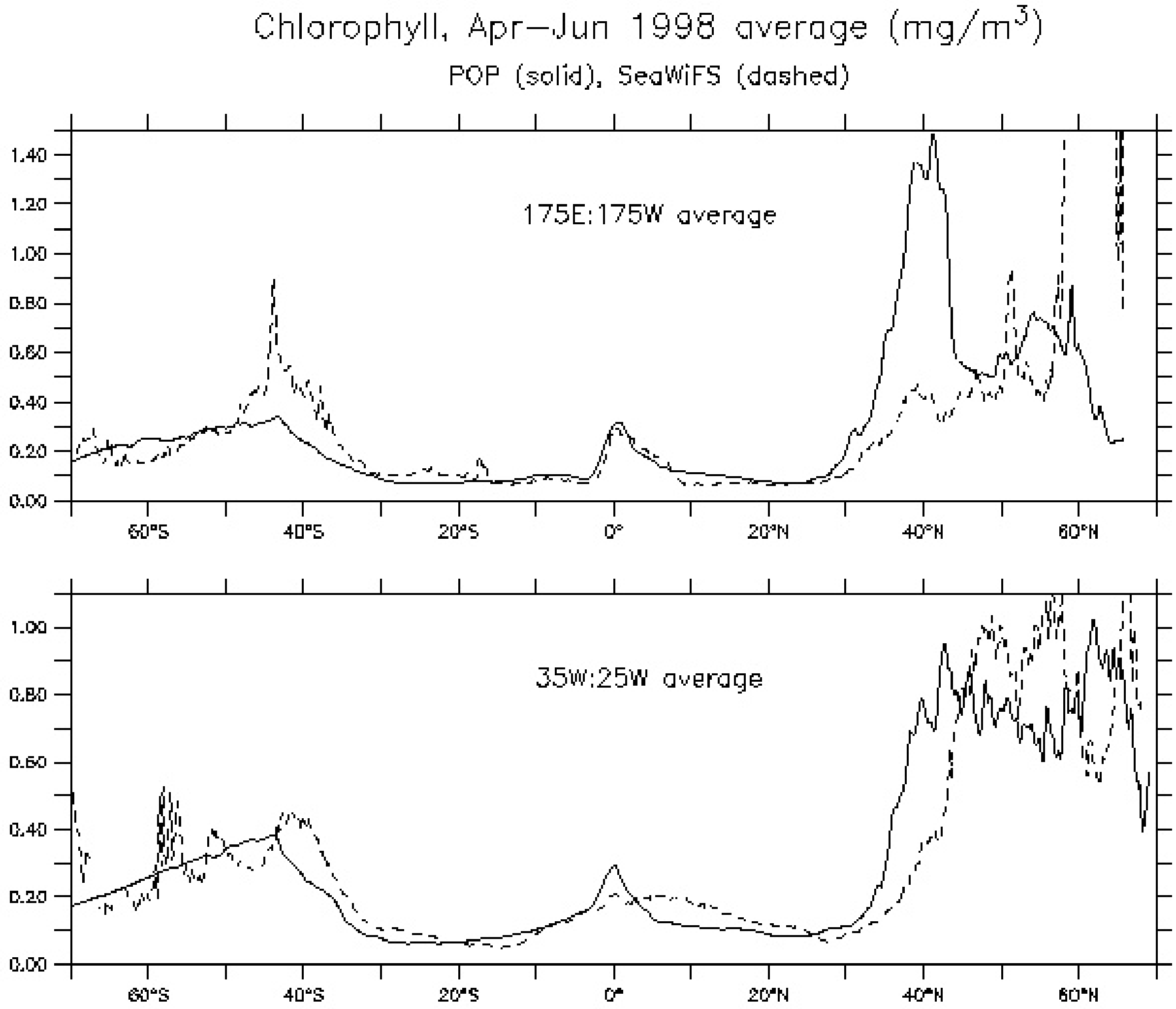
BACKGROUND



- COSIM founded on POP and CICE
- Performance, portability, fine resolution - LANL codes now the core of CCSM
- Biogeochemistry relatively new -global ecosystems, trace gases
- All agree high latitudes are the next wave
- Warming fastest, understudied -ice loss/change, sensitive biota

Comparison with SeaWiFS Chlorophyll



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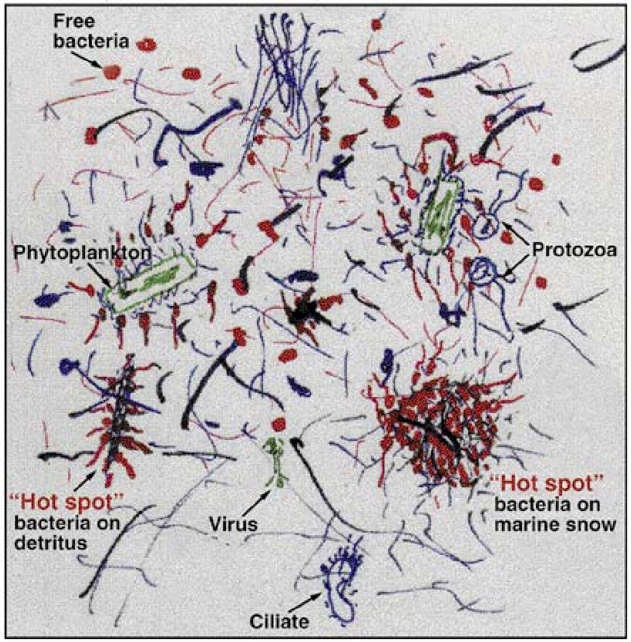
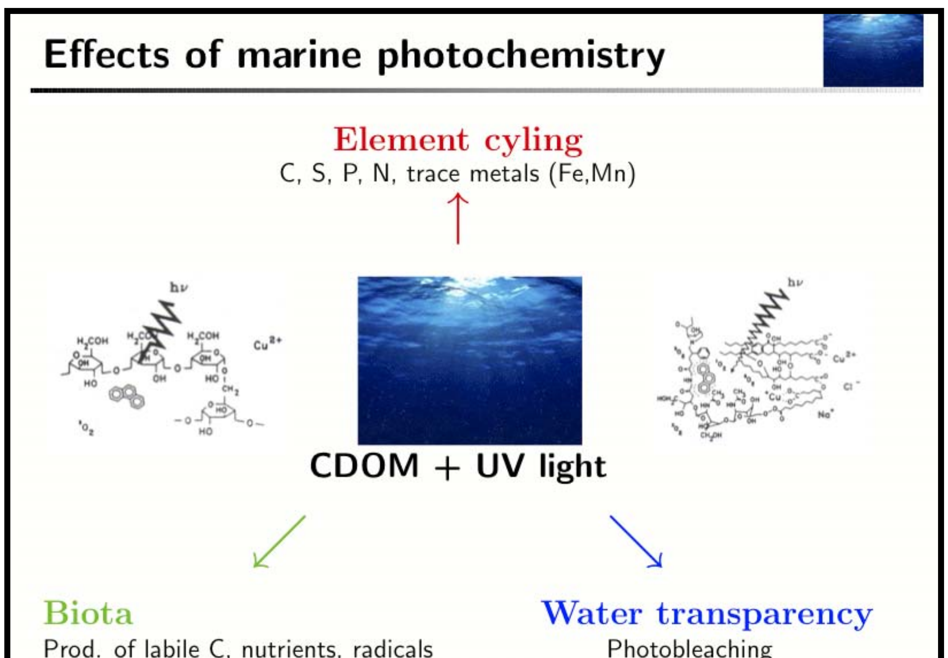
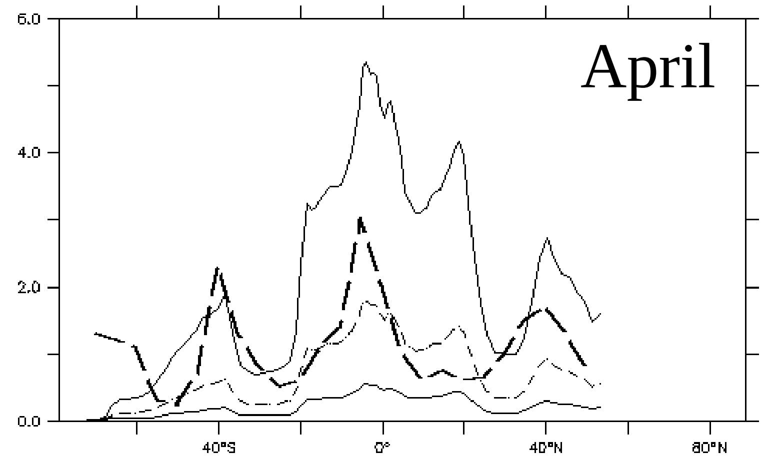
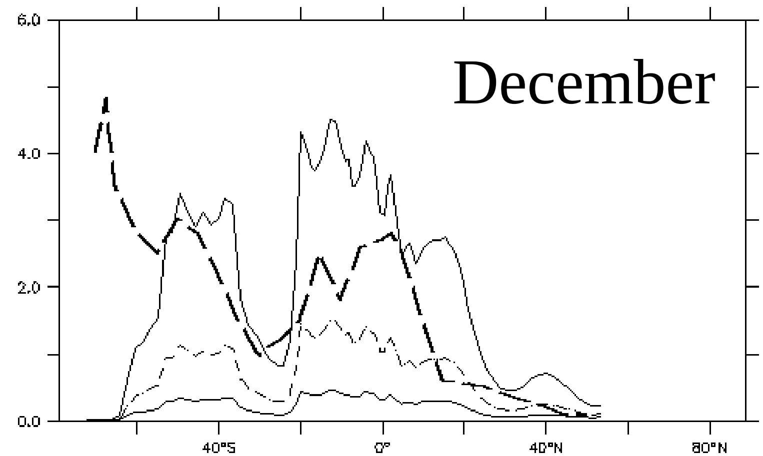
Carbon Monoxide

- •CDOM interacts with UV
- •PMEL cruises at 140W
- •POP quantum yield test

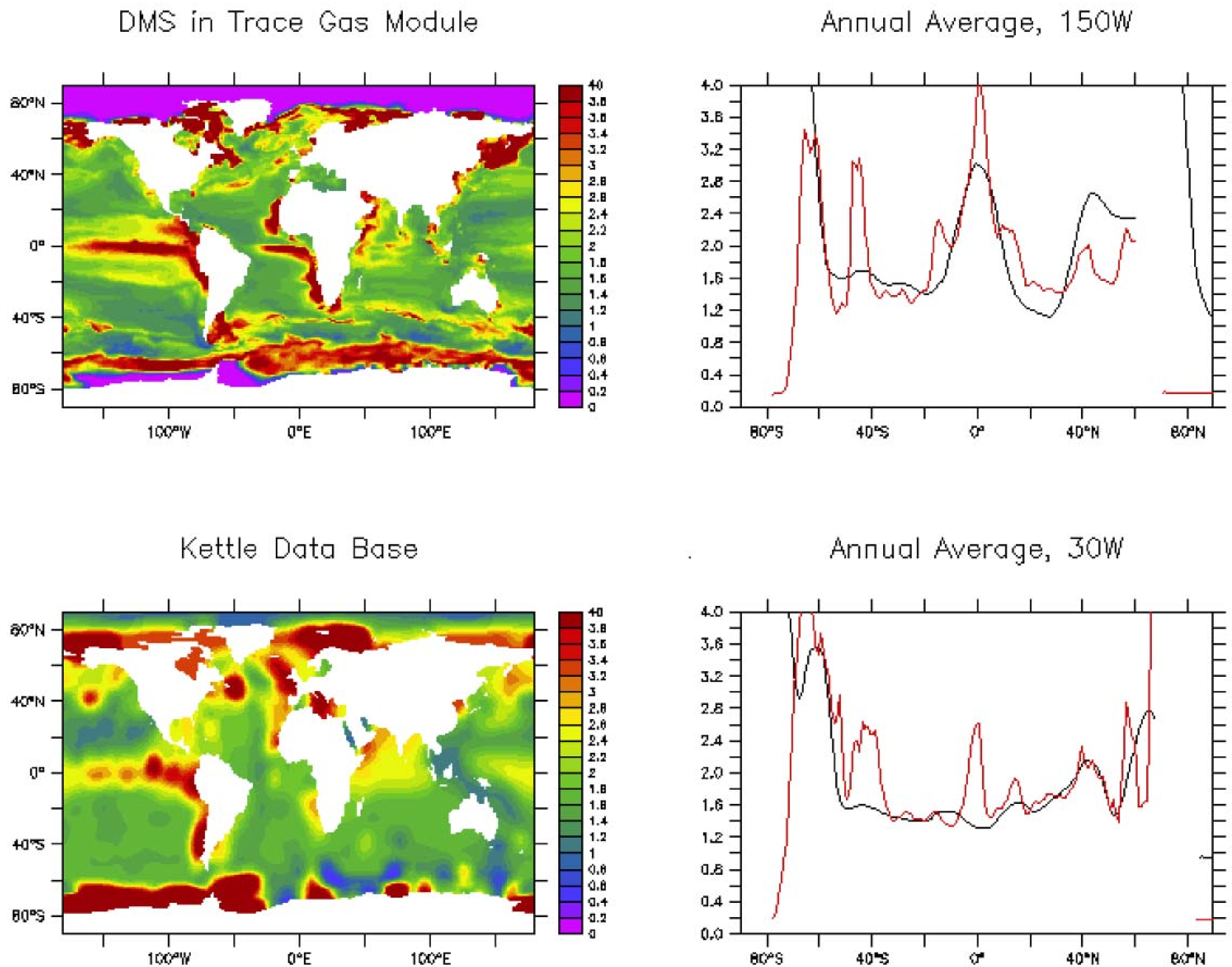




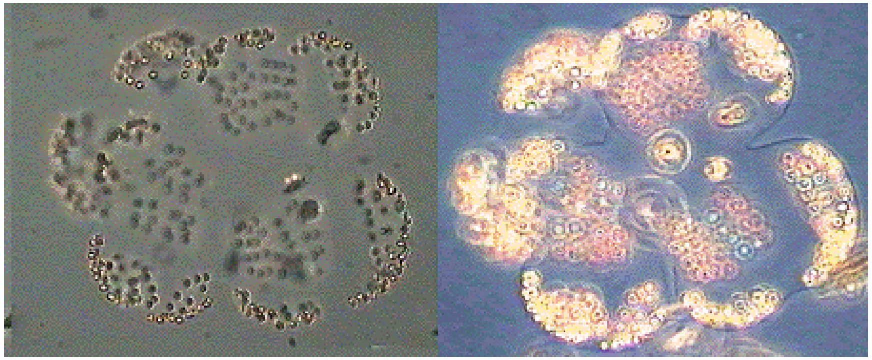




Dimethyl Sulfide (nM) Year 33, LM86 Piston Velocity



WINTERIZE GEOCYCLING



- Interest originates with pigment, DMS and photochemistry problems
- Elect to improve polar S cycle first
- Develop code for new organisms, ecosystems and processes
- Note high latitudes clearly are the next wave for all of COSIM

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TODAY'S EXAMPLE: ICE ALGAL DEMO

- CICE is global in the sense that ice simulated both hemispheres
- But we will focus here on Arctic -timely and biology simpler
- Demonstration of capability only at this point
- Work from landfast models -Arrigo, Lavoie (Denman), Jin (Deal)
- Relatively well documented, convergent, between them inclusive
- Skeletal layer only and decoupled from POP
- Key inputs: CICE radiative transfer, hv and Si limits, melt removal
- Key results: cryobiology driven by light, snow cover and melt rate

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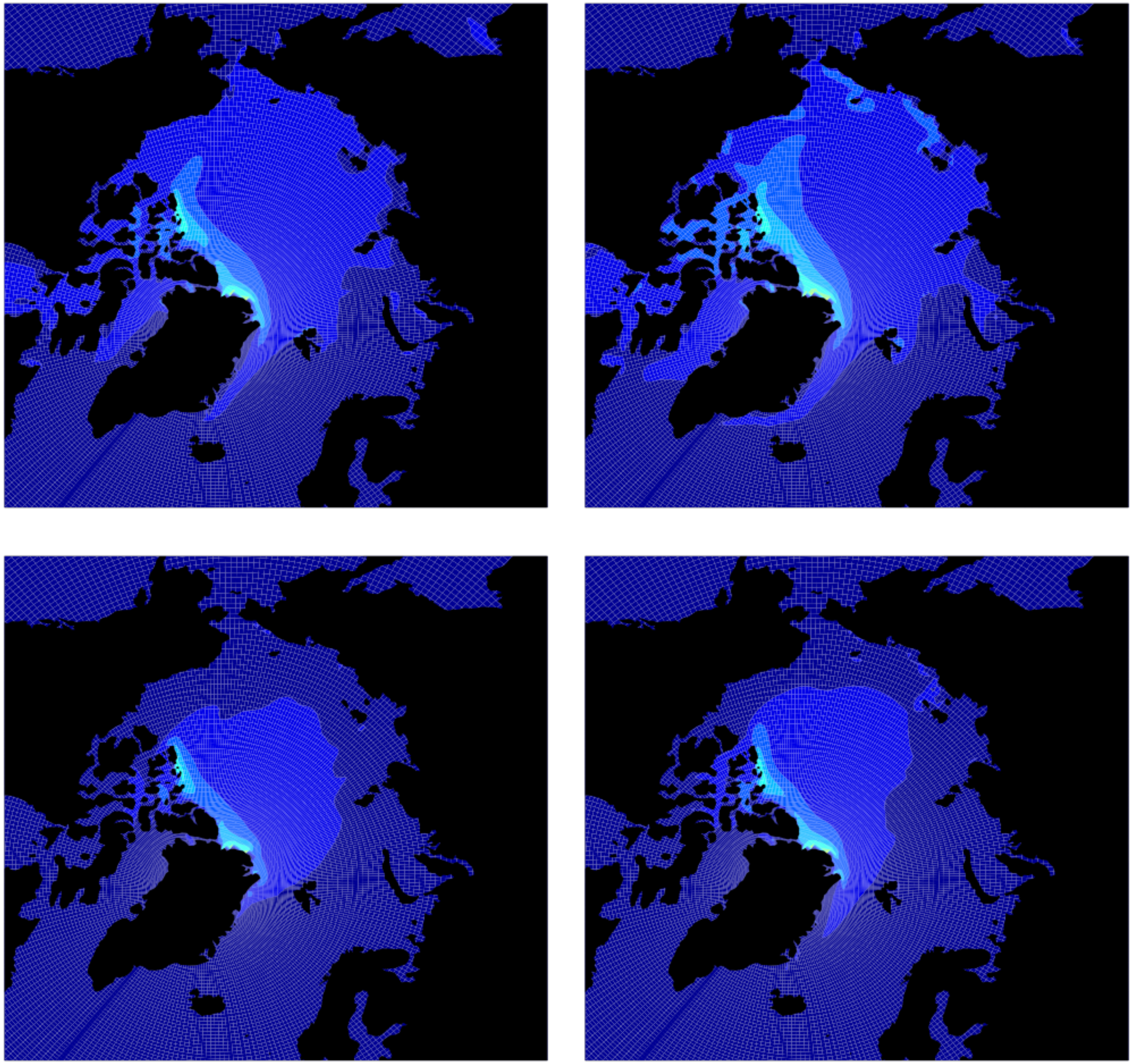
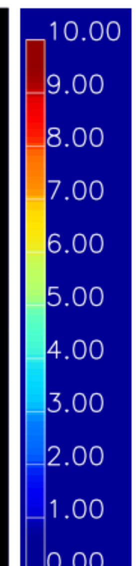
Ice Thickness

Feb May
Aug Nov

Units -meters

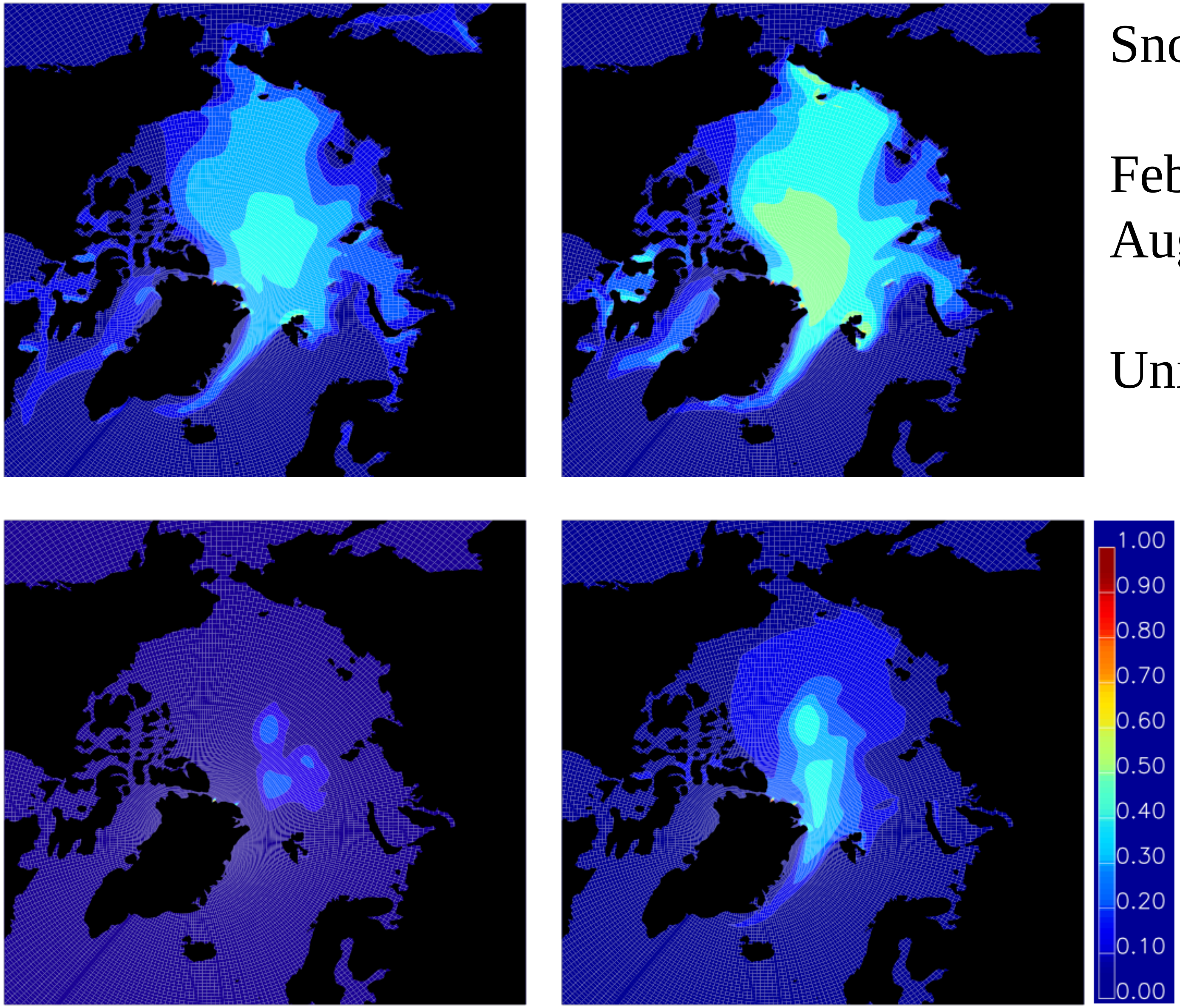




Snow Cover

Feb May
Aug Nov

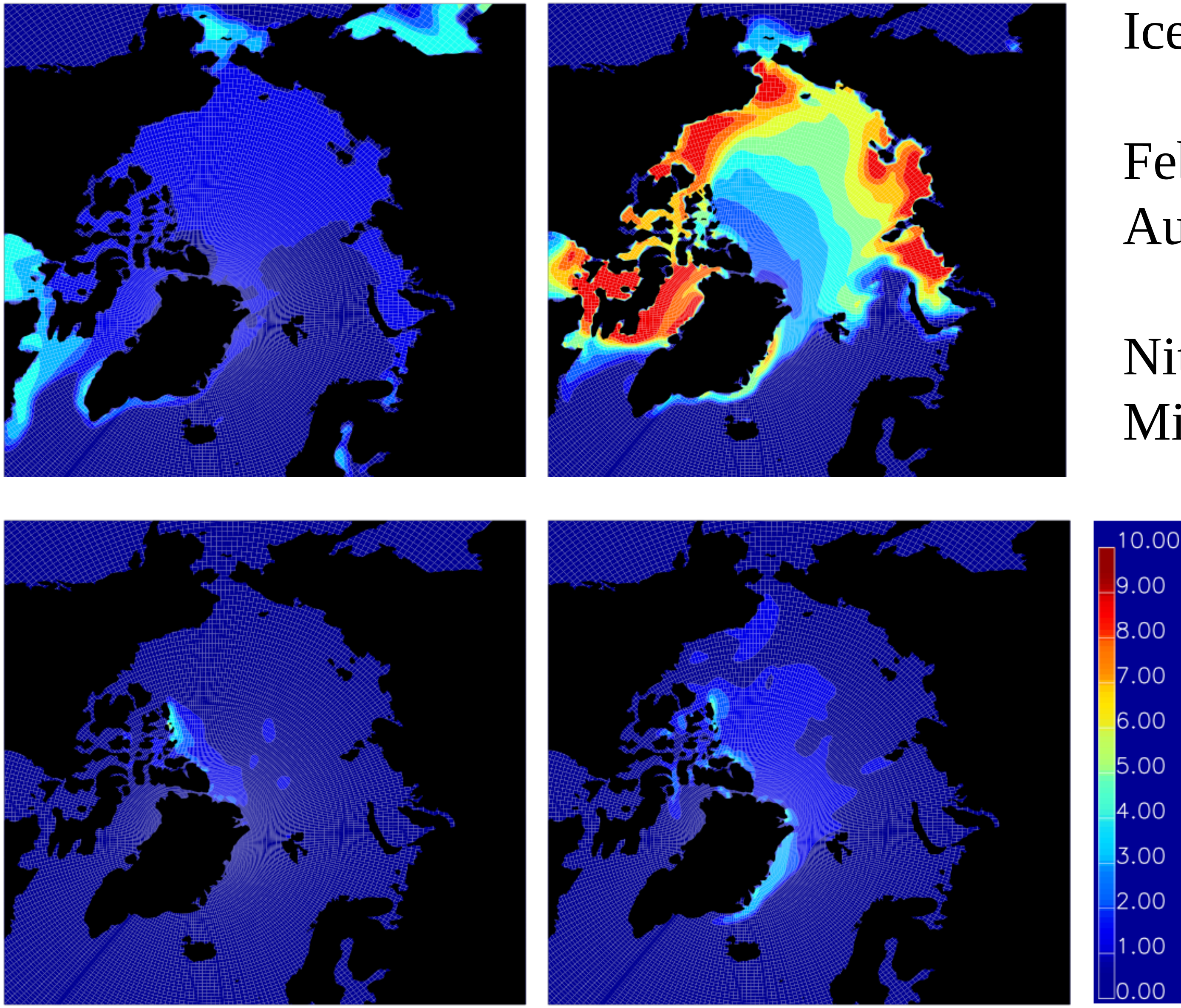
Units -Meters



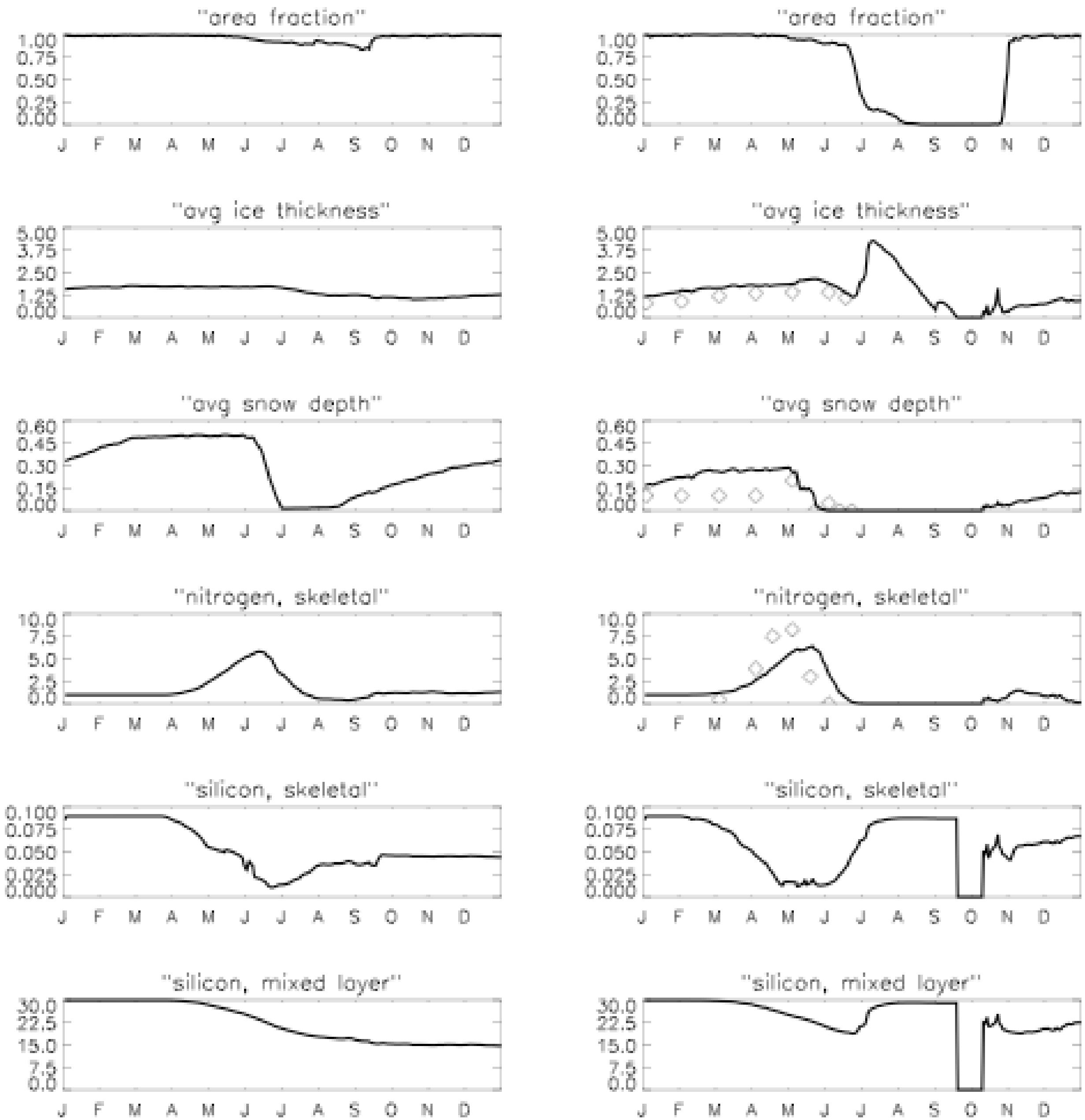
Ice Algae

Feb May
Aug Nov

Nitrogen,
Millimoles/m2



Pole | Barrow



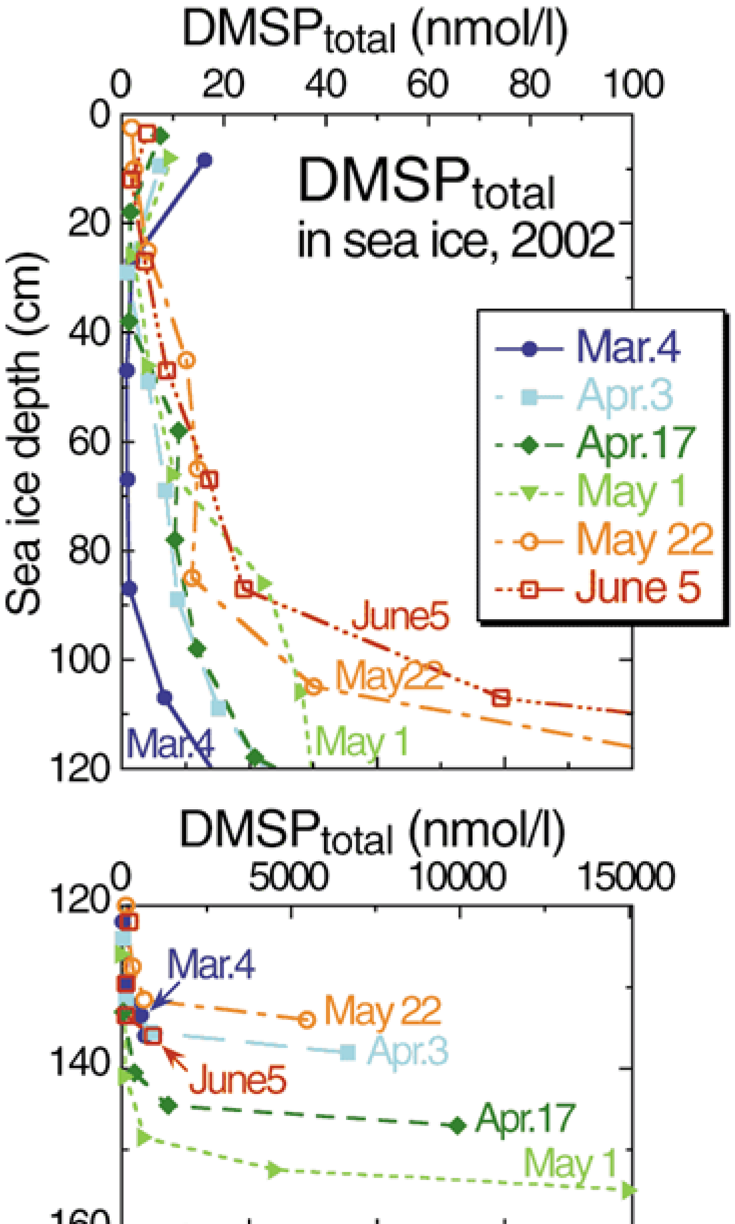
Units:

Length - meters

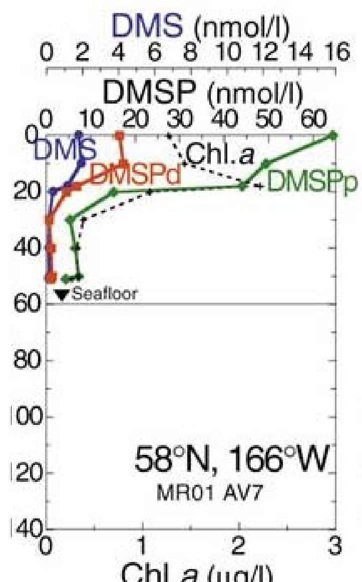
Concentration - Millimoles/m2

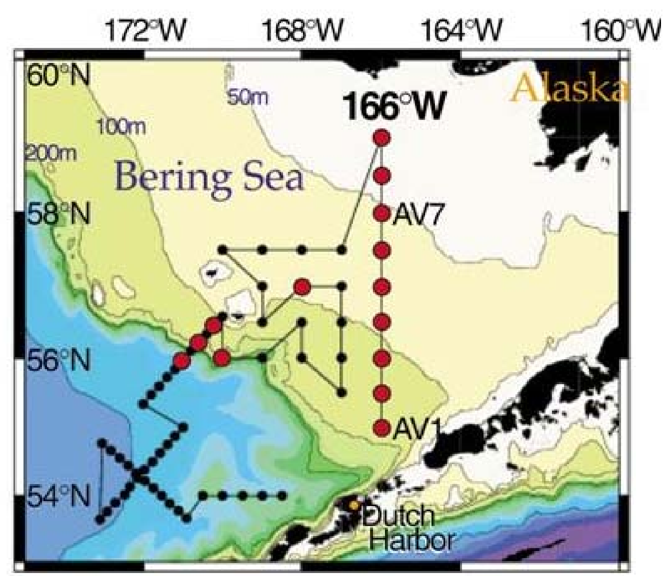
ON TO COLLABORATIONS

- Framework is ready
- Harvest data, guidance, assistance
- Several groups have S and other results
- Build 1st regional DMS ice model
- Multielemental basis has to be strong



Offshore Barrow, Landfast



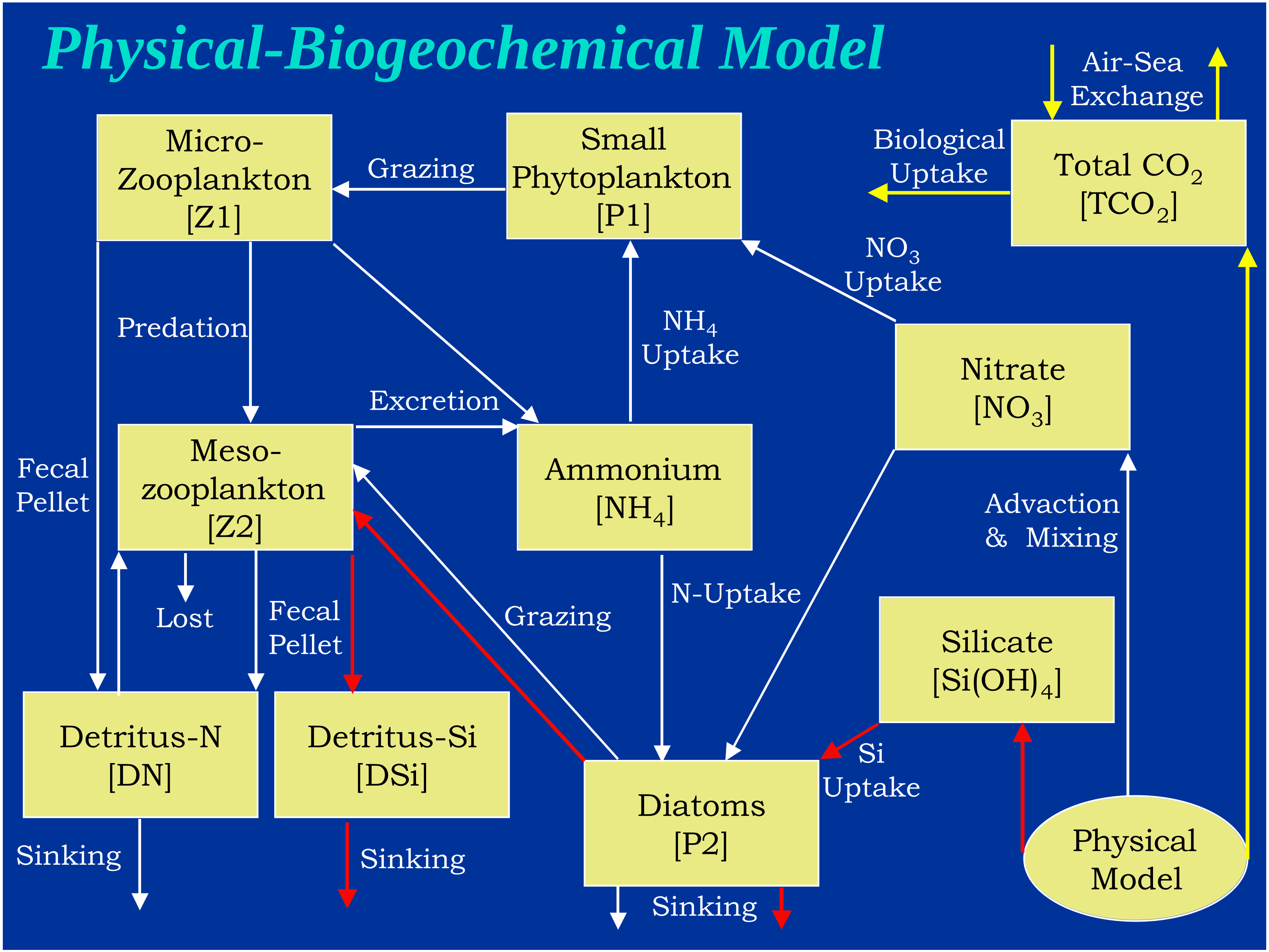


Water column Bering
All data courtesy Deal IARC

HIGH LATITUDE BIOGEOCHEMISTRY PLANS

- **NEAR TERM:**
- **Read up on Walsh, Arrigo foundation models and all data sets**
- **Add N limitation and a sulfur mechanism within CICE**
- **MEDIUM TERM:**
- **Link to POP geocycling and CICE radiative transfer**
- **LONGER:**
- **Expand to include Antarctic**
- **Include high latitude specialists in biogeochemical POP**
- **Ultimately systems simulations of (bi) polar geochemical change**

EXTRAS 1


Physical-Biogeochemical Model
Air-Sea Exchange
Micro-Zooplankton [Z1]
Grazing
Small Phytoplankton [P1]
Biological Uptake
Total CO_2 [TCO_2]
NO_3 Uptake
Predation
NH_4 Uptake
Nitrate [NO_3]
Excretion
Meso-zooplankton [Z2]
Ammonium [NH_4]
Fecal Pellet
Advaction & Mixing
Lost
Fecal Pellet
Grazing
N-Uptake
Silicate [$Si(OH)_4$]
Detritus-N [DN]
Detritus-Si [DSi]
Si Uptake
Diatoms [P2]
Physical Model
Sinking
Sinking
Sinking

Plankton Dynamics

Rates

$$V_p = 0.6\left(1.066^T\right),\quad (1-4)d^{-1}$$

$$J(z) = \frac{V_p \alpha I(z)}{\left(V_p^2 + \alpha I(z)^2\right)^{1/2}},\quad \frac{-dI(z)}{dz} = \left(k_w + k_p Chl\right)$$

$$SMS(N_p) = (1-\gamma_1)J(z)[Q_1 + Q_2]N_p - G_1 - \mu N_p$$

$$SMS(N_z) = \gamma_2(G_1 + G_2 + G_3) - (\mu_2 + \mu_5)N_z$$

$$Q_1 = N_n e^{-\psi N_r} / (K_1 + N_n)$$

$$Q_2 = N_r / (K_1 + N_r)$$

$$G_1 = gN_z \frac{p_j C_j}{K_3 + \sum p_k C_k},\ j,k = 1...3$$

Fasham et al. 1990, 1993
Sverdrup, Johnson & Fleming 1942

Enzyme, predator-prey
and other kinetic types

System

***SMS** (other P, Z, B, DOM, POM with sedimentation)*
Then other elements carbon, silicon, phosphorus, iron…
And what about steady states?

Conserve atoms
but not energy…

Compensation

$$I_c = I \text{ for photosynthesis} = \text{respiration, typically} \sim 0.1P_{\max}$$

$$P_{gross} = P_{\max} I / (I_{1/2} + I)$$

$$V_p = \alpha I_{1/2}, V_p = 3d^{-1}, \alpha = 0.03\left(1/dw/m^2\right), I_{1/2} = 100w/m^2, I_c \sim 20w/m^2$$

Attenuation

$$I(z) = I_o e^{-(k_w + k_p Chl)z}, k_w = 0.03m^{-1}, k_p = 0.03\left(1/mg/m^3\right), \overline{I_o} = 100w/m^2, z(c) = 50m$$

$$\overline{I_D} = \frac{1}{D}\int_0^D I_o e^{-kz} dz, \frac{I_o}{Dk}\left(1 - e^{-kD}\right) \quad \text{average to } D$$

Criticality

$$D_{cr} = \frac{I_o}{I_c k} \text{ if } kD_{cr} >> 0, D_{cr} \sim 150m$$

Mixing must remain <D_{cr} for net growth

Landfast Ice Conceptual Models

Antarctic

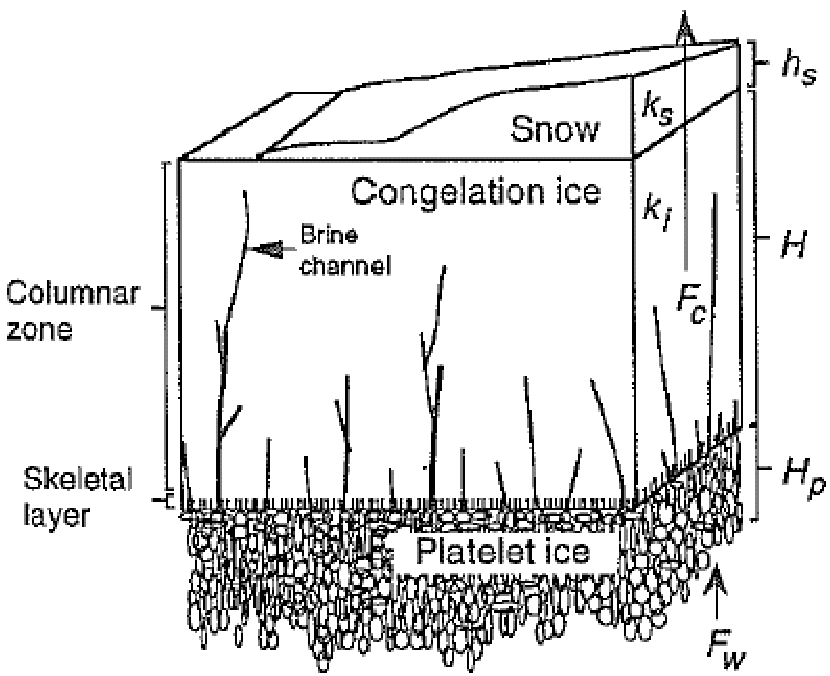


Fig. 1. Sea ice growth model. Separate terms represent the temperatures (degrees Celsius) of the air (T_a), upper sea ice or snow surface (T_o), sea ice interior (T_i), and lower sea ice surface (T_f), which is also equivalent to the freezing point of seawater. H and h_s refer to the thicknesses of the sea ice and snow (meters), respectively, while the conductive flux of heat through the sea ice is denoted by F_c, and the flux of heat from the seawater by F_w. The thermal conductivity of sea ice and snow are denoted by k_i and k_s, respectively. By convention, all fluxes into the sea ice, such as F_w, are positive, and all fluxes out of the ice sheet, such as F_c, are negative.

Arctic

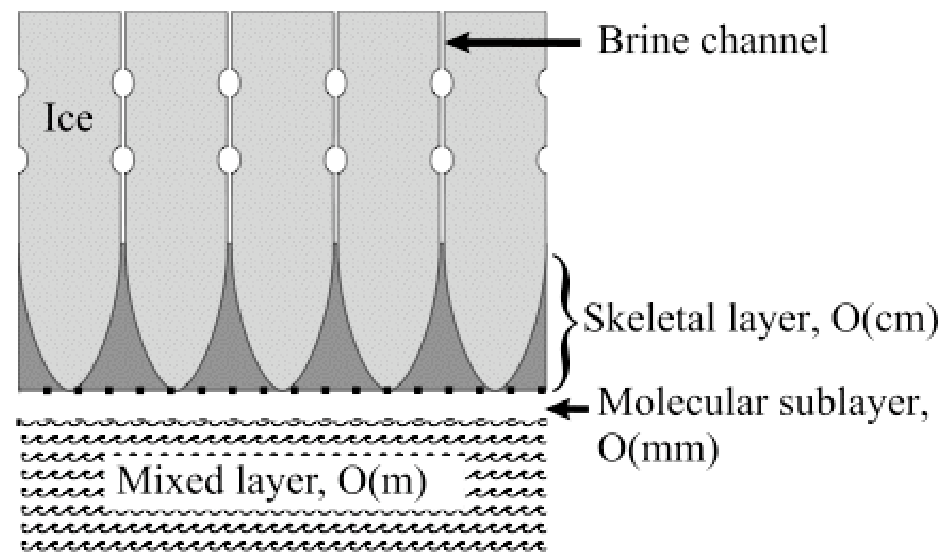


Figure 2. Schematic of the different layers at the base of the ice (light gray). Ice algae (dark gray) are found in the skeletal layer.

Landfast Ice Chlorophyll Profiles

Antarctic

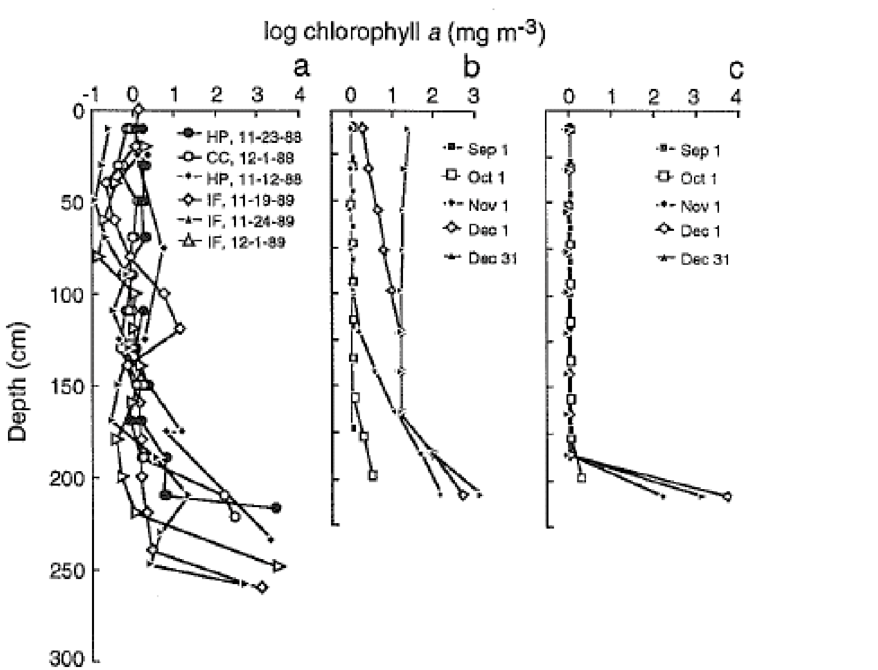


Fig. 10. (a) Vertical chlorophyll *a* profiles from congelation ice cores collected in McMurdo Sound, Antarctica, during 1988 an 1989, and simulated vertical chlorophyll *a* distributions assuming that (b) $g(z)=0$ throughout the congelation ice or (c) that $g(z)=$ in the upper layers of the congelation ice and $g(z)=0$ in the lower layers.

Arctic

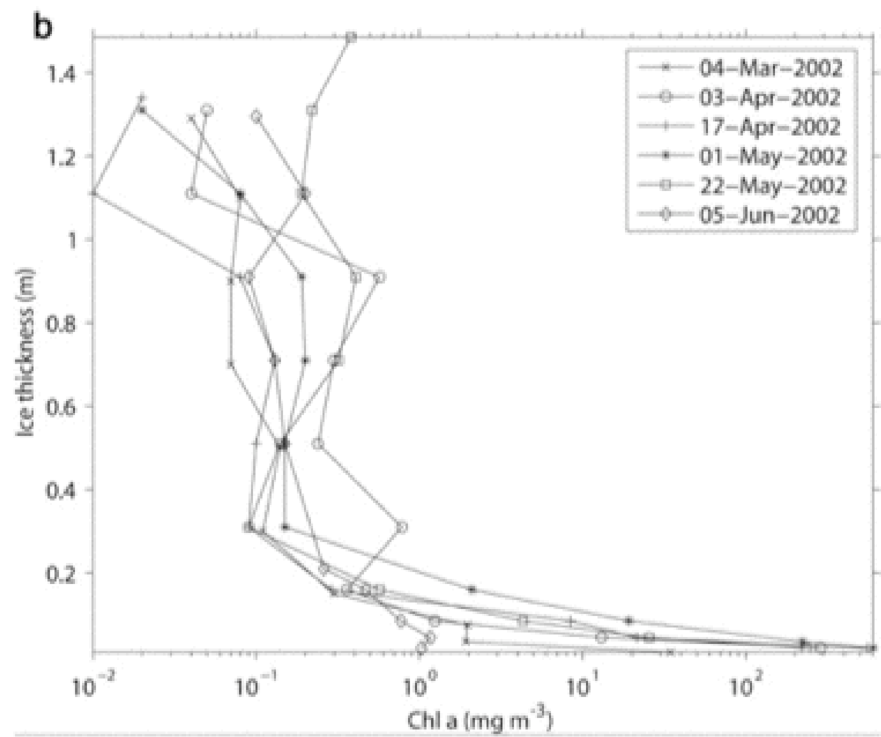


Fig. 3. Observed (a) ice temperature and (b) ice-algae distribution in sea ice at IARC site in 2002.

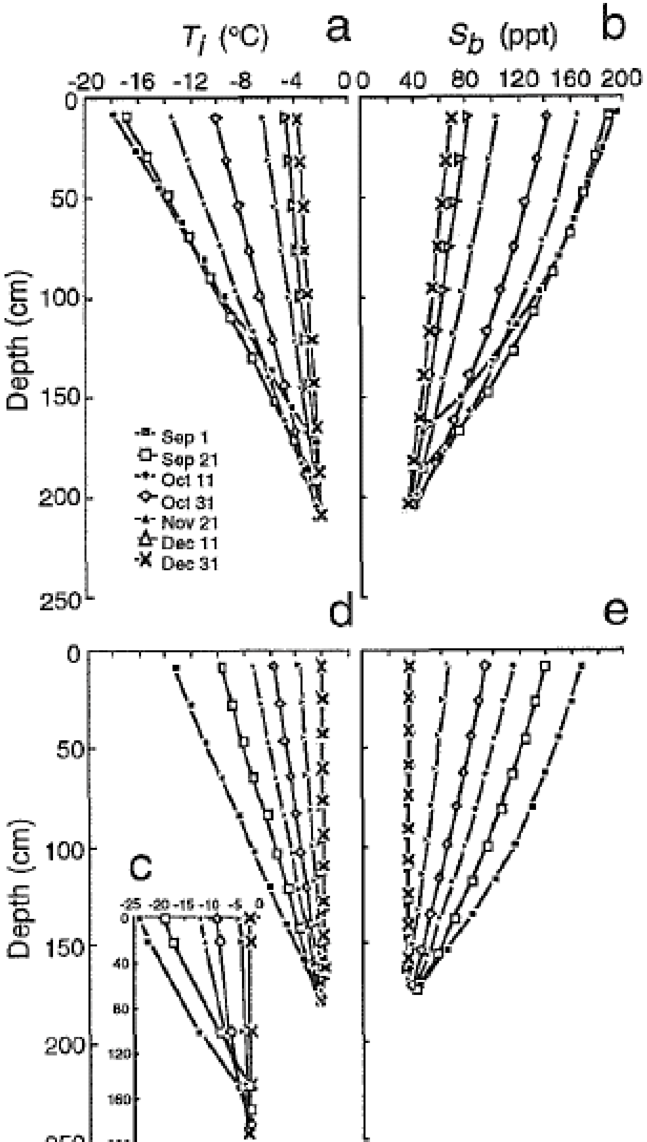


Fig. 6. Time series of simulated temperature, $T_i(z)$, and brine salinity, $S_b(z)$, profiles in congelation ice. Figures 6a and 6b correspond to run 2 (mean temperature) and Figures 6d and 6e to run 11 (high temperature). Figure 6c is time series of observed sea ice temperature profiles measured with a copper canstantan thermistor chain in McMurdo Sound, Antarctica,

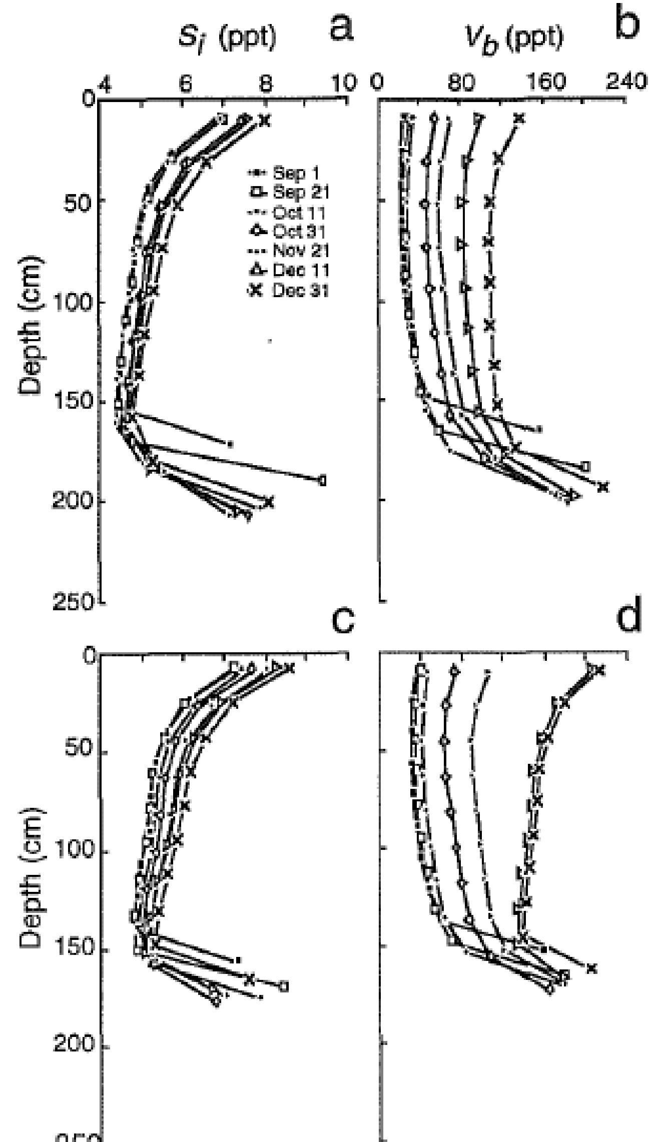


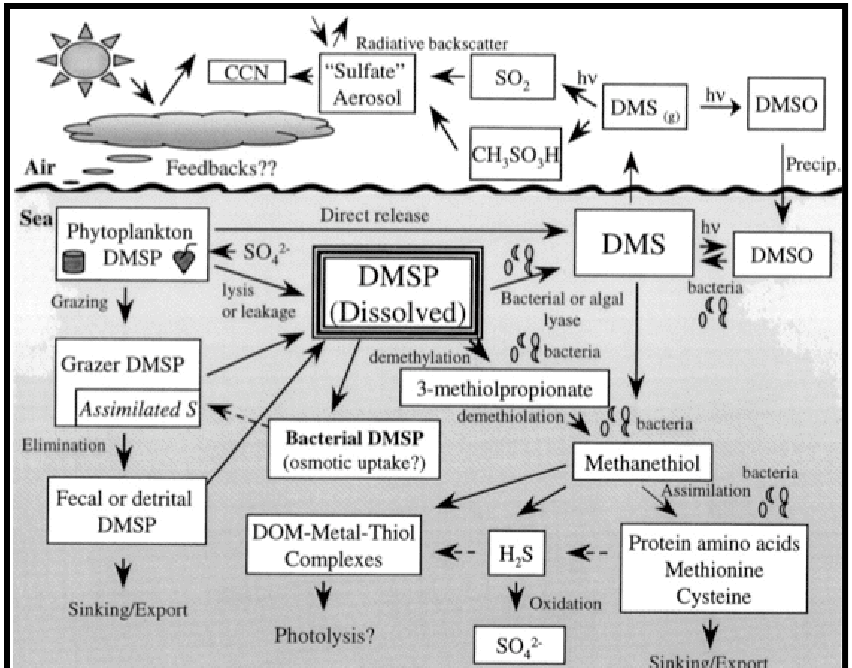
Fig. 7. Time series of simulated sea ice salinity, $S_i(z)$, and brine volume, $V_b(z)$, profiles in sea ice. Figures 7a and 7b correspond to run 2 (mean temperature) and Figures 7c and 7d to run 11 (high temperature).

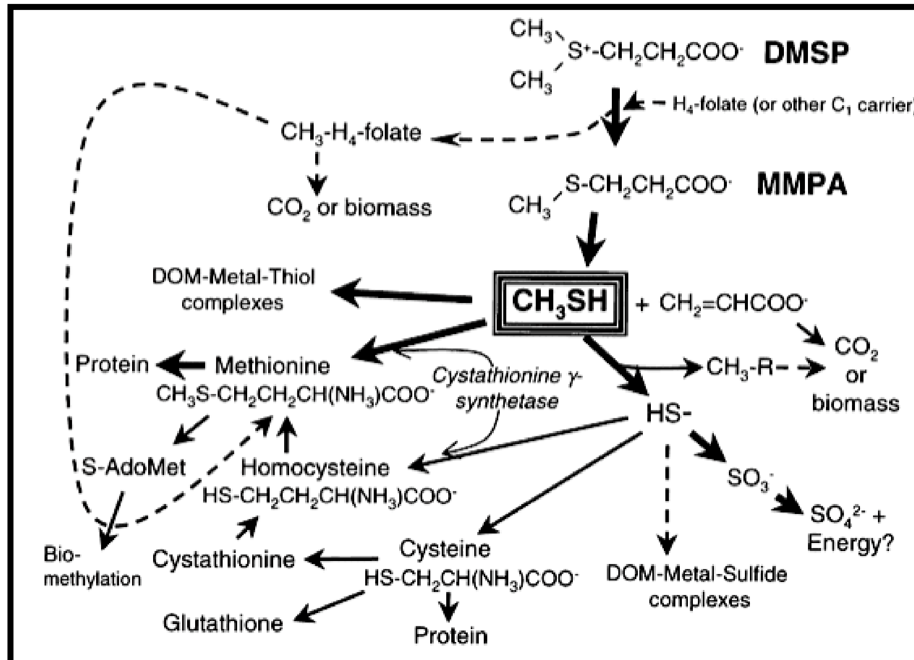
DMS BIOGEOCHEMISTRY

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}

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





Assimilation to DMSP

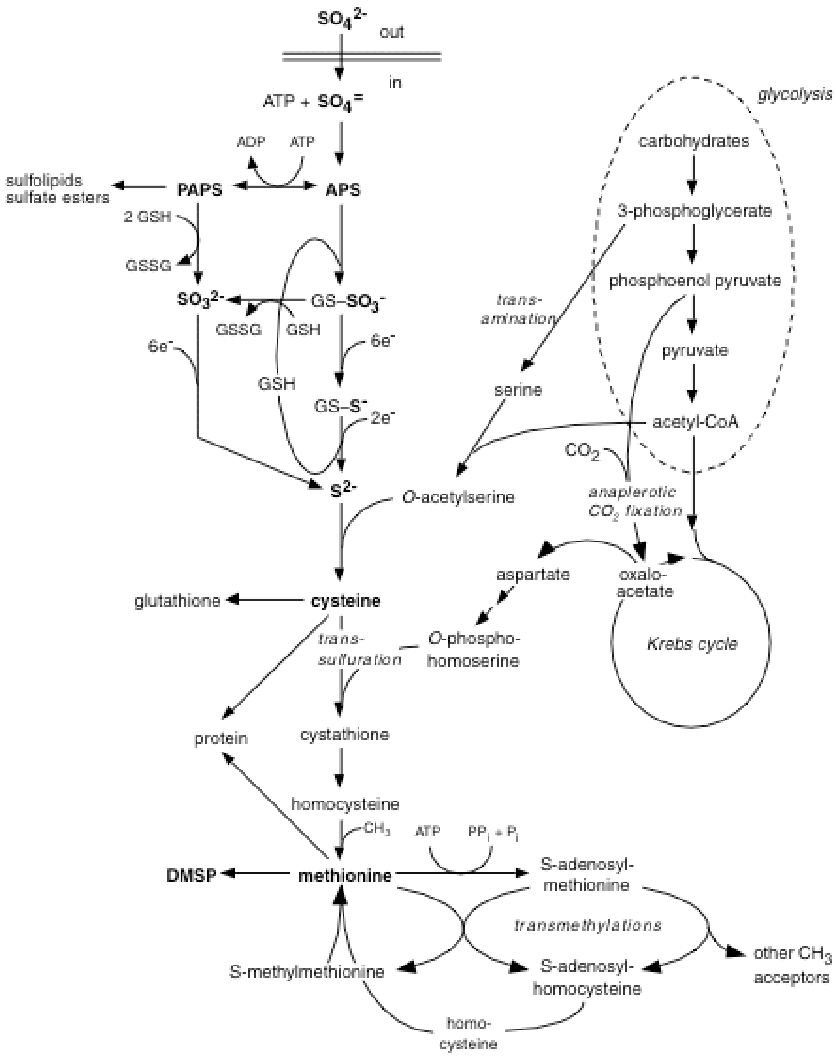


Fig. 1. Schematic representation of the processes involved in the assimilatory sulphate reduction and biosynthesis of DMSP. No attempt has been made to represent stoichiometries. Explanation is given in the text. This figure is extracted from references discussed in the text and from Quispel and Stegwee (1983) and Salisbury and Ross (1992).

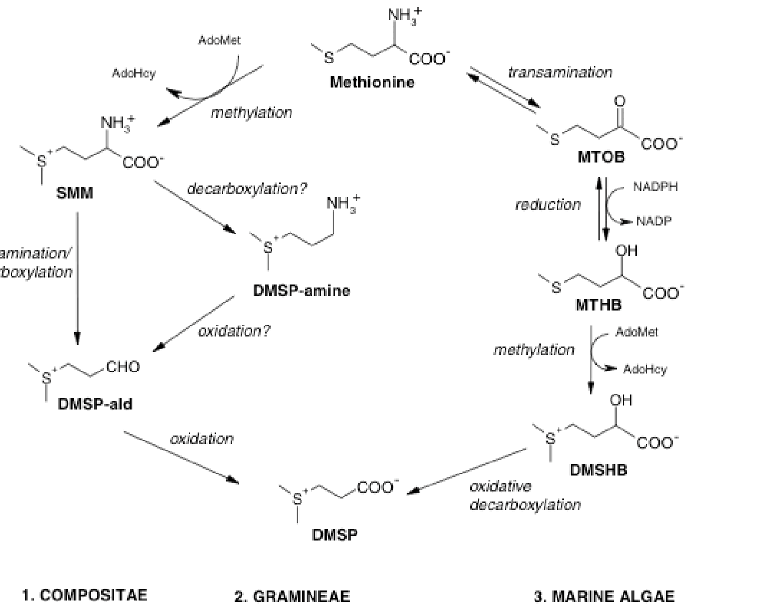


Fig. 2. Schematic representation of the three pathways of DMSP biosynthesis from methionine (after Hanson and Gage, 1996; Gage et al., 1997; Kocsis et al., 1998; Summers et al., 1998).

Phaeocystis DMSP as f(S)

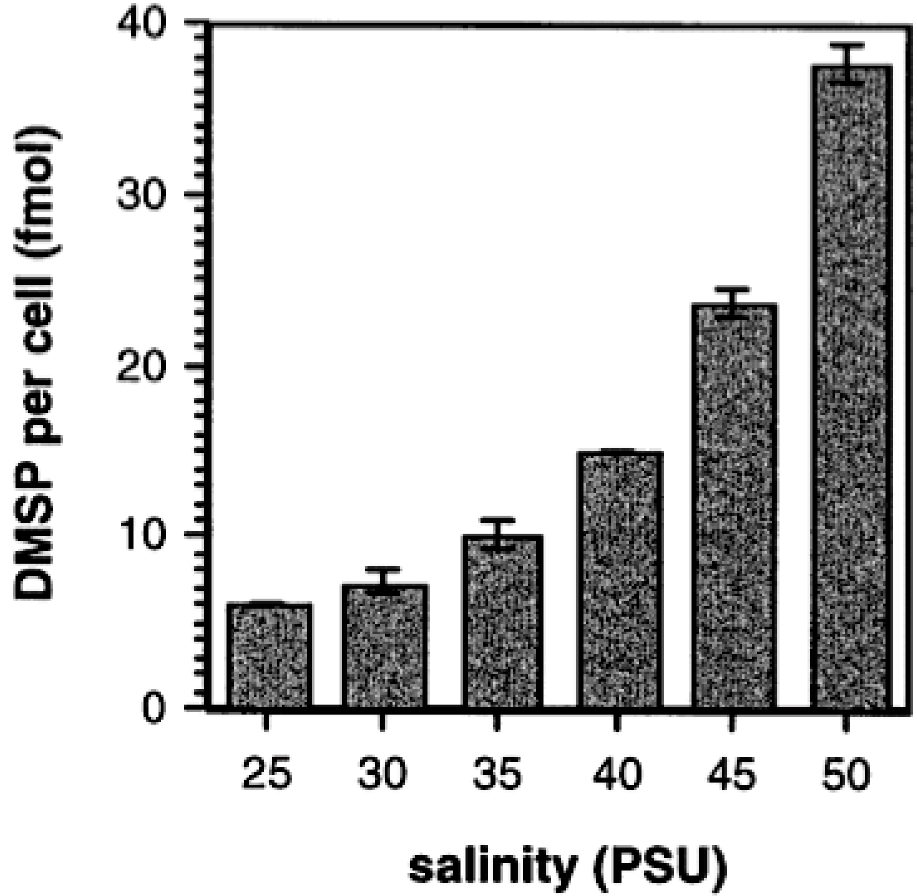
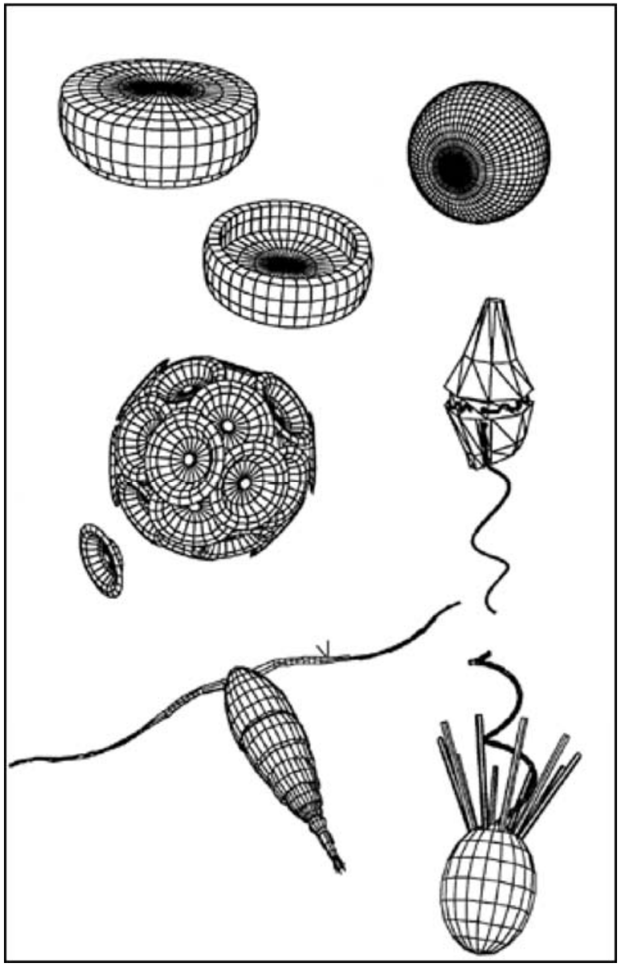


Fig. 3. DMSP content of *Phaeocystis* sp. cells growing exponentially in batch cultures. Cells were adapted to the salinities for at least five generations. Values are means of duplicate cultures; range is indicated.

Some Biogeochemical POP History

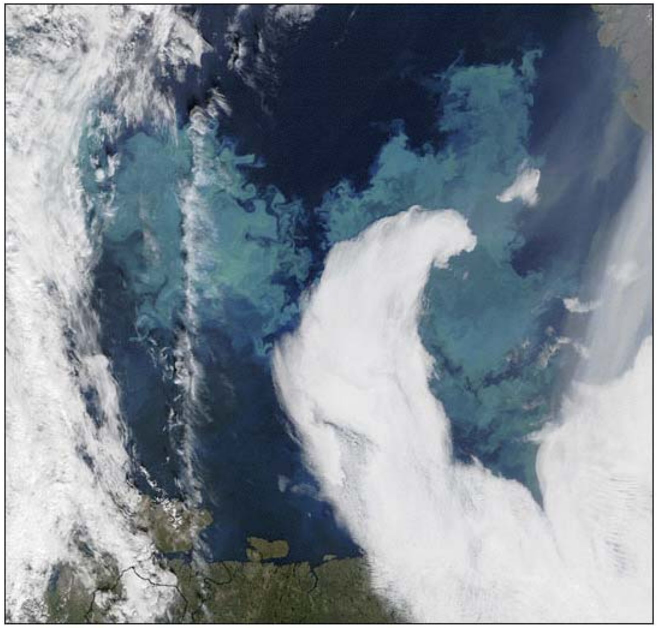


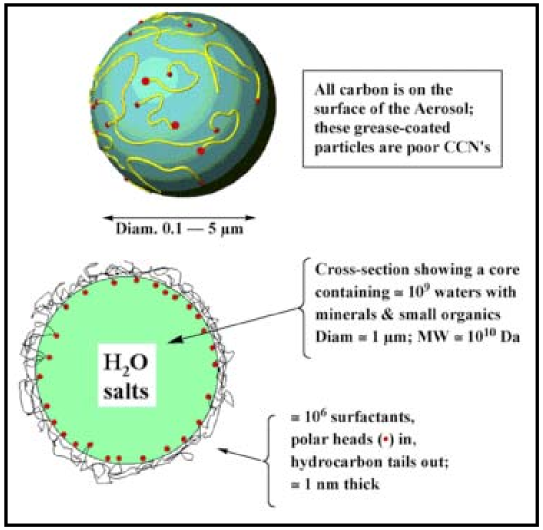
- Earth System Modeling became COSIM focus

- Global change begins with CO2 but loops back onto all of ecology and elemental cycling

- Hence biogeochemistry unavoidable

- Mainstays have been fine grids, Fe fertilization, and the climate active trace gases





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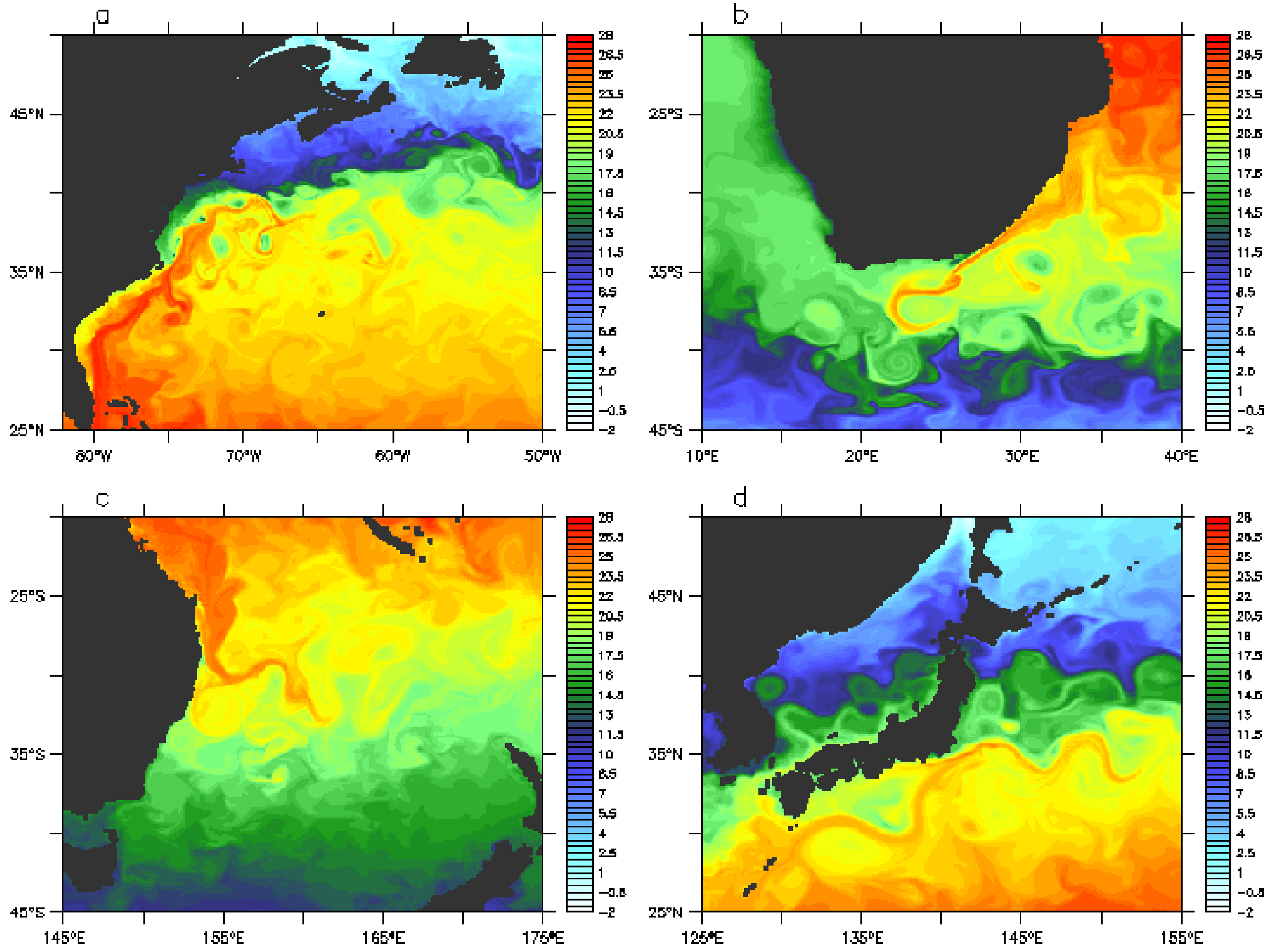
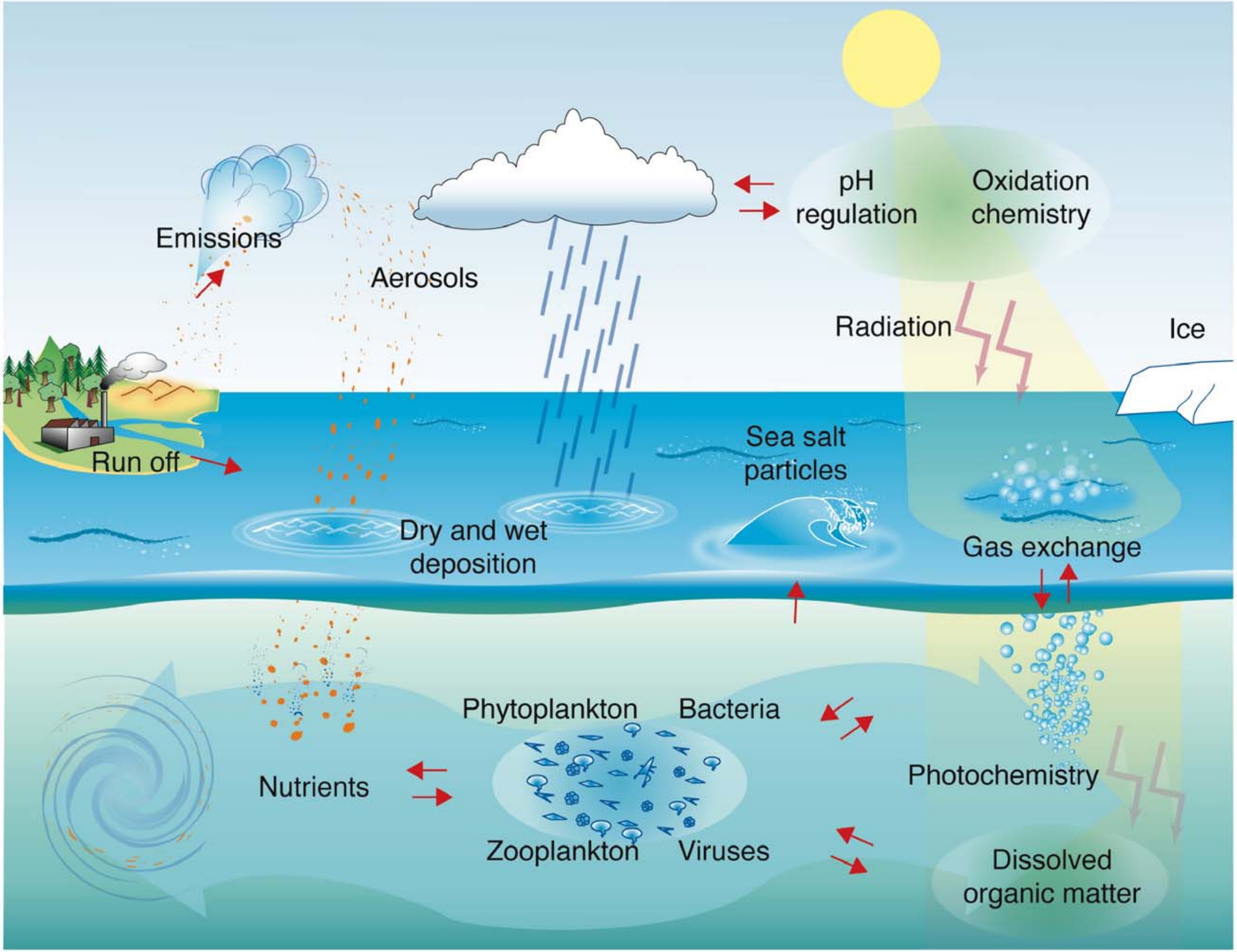
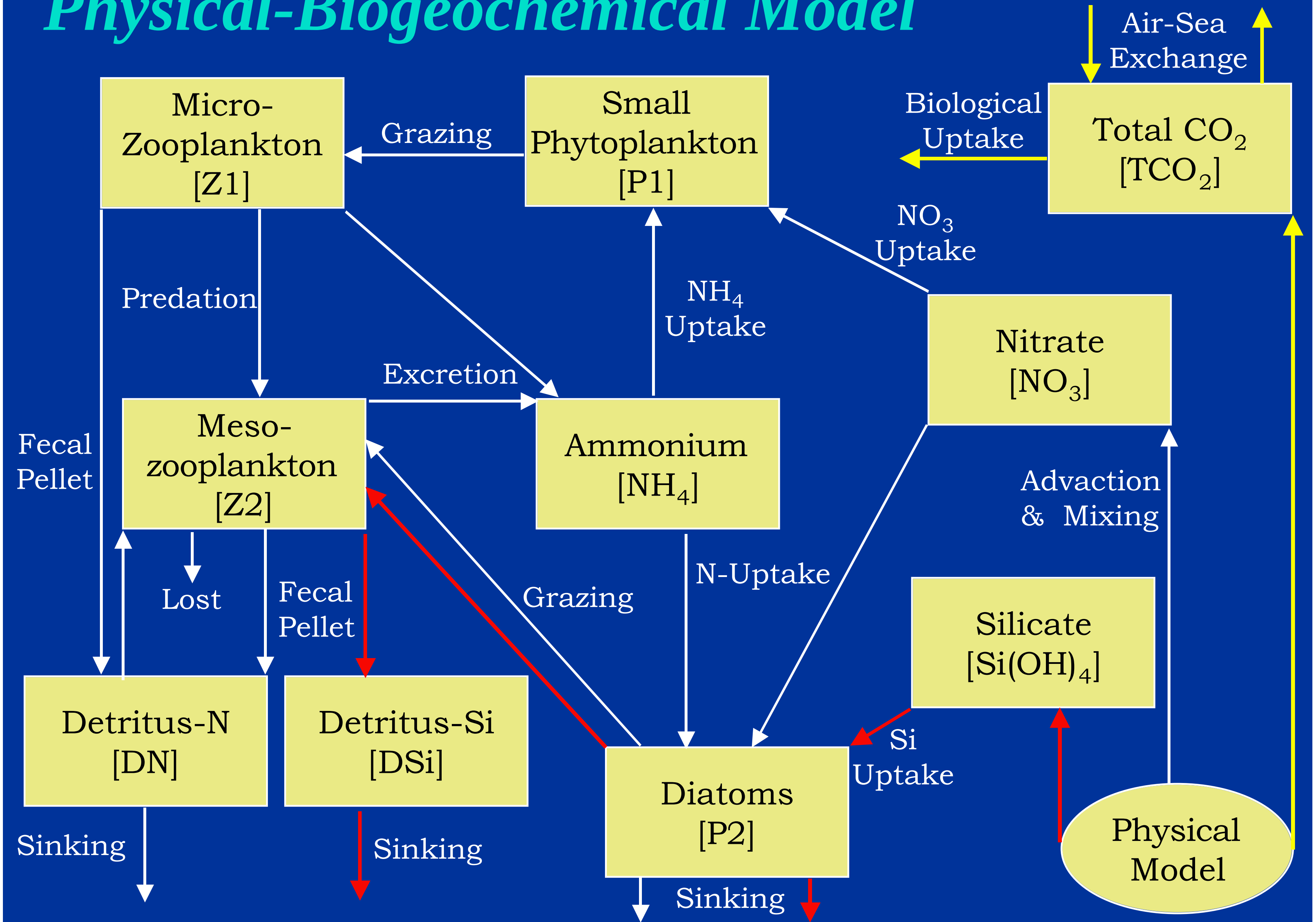
POP Physics Simulations



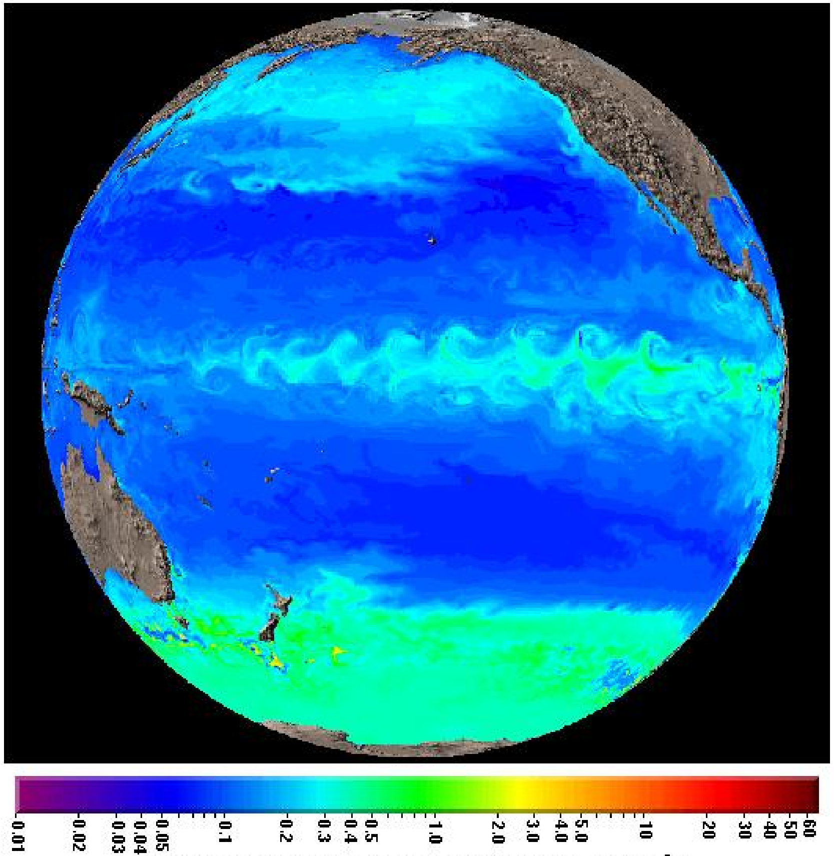


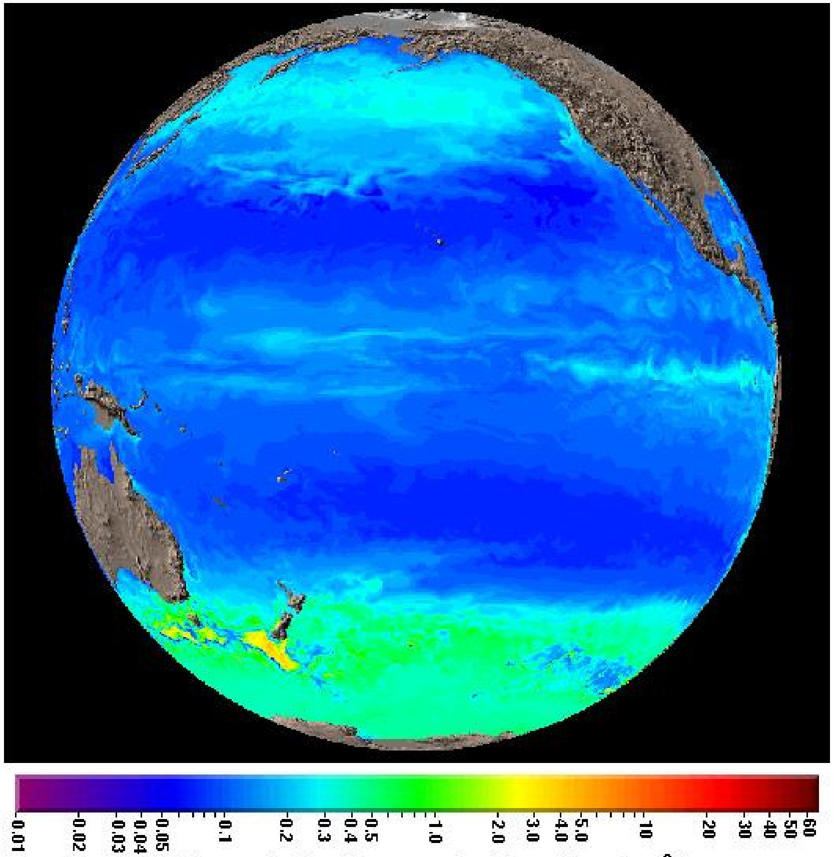
Emissions
Aerosols
pH regulation
Oxidation chemistry
Radiation
Ice
Run off
Sea salt particles
Dry and wet deposition
Gas exchange
Phytoplankton
Bacteria
Nutrients
Photochemistry
Zooplankton
Viruses
Dissolved organic matter

Physical-Biogeochemical Model



Simulation of a La Niña to El Niño Transition





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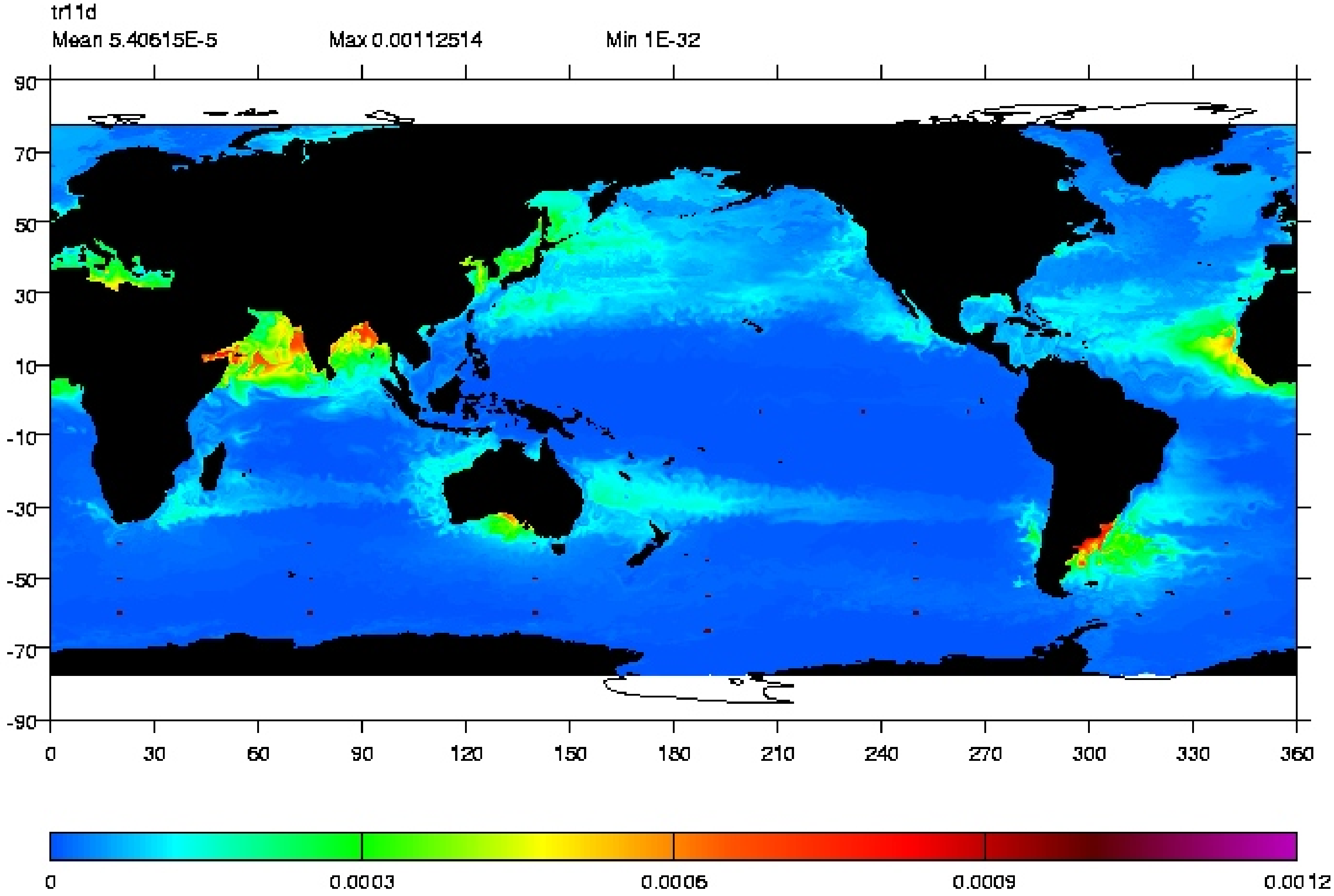
Initial Southern Hemisphere Patch Positions and Iron Background (μM)



/am/nearstore1/vol/vol2/ice-bio/spchu/1280_18tracer/bf.set/movies/patch/mfp1.11 b.74461.nc

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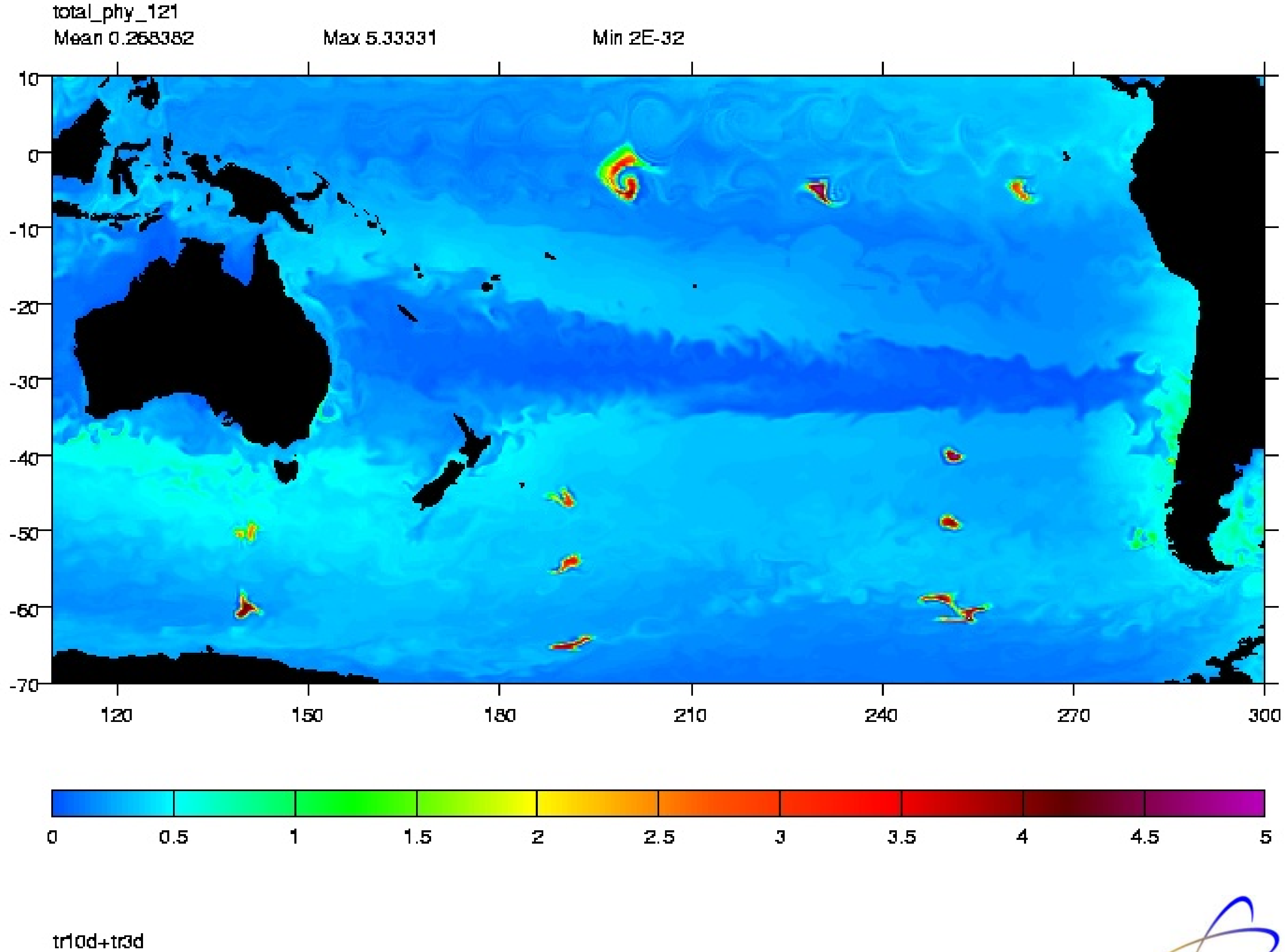
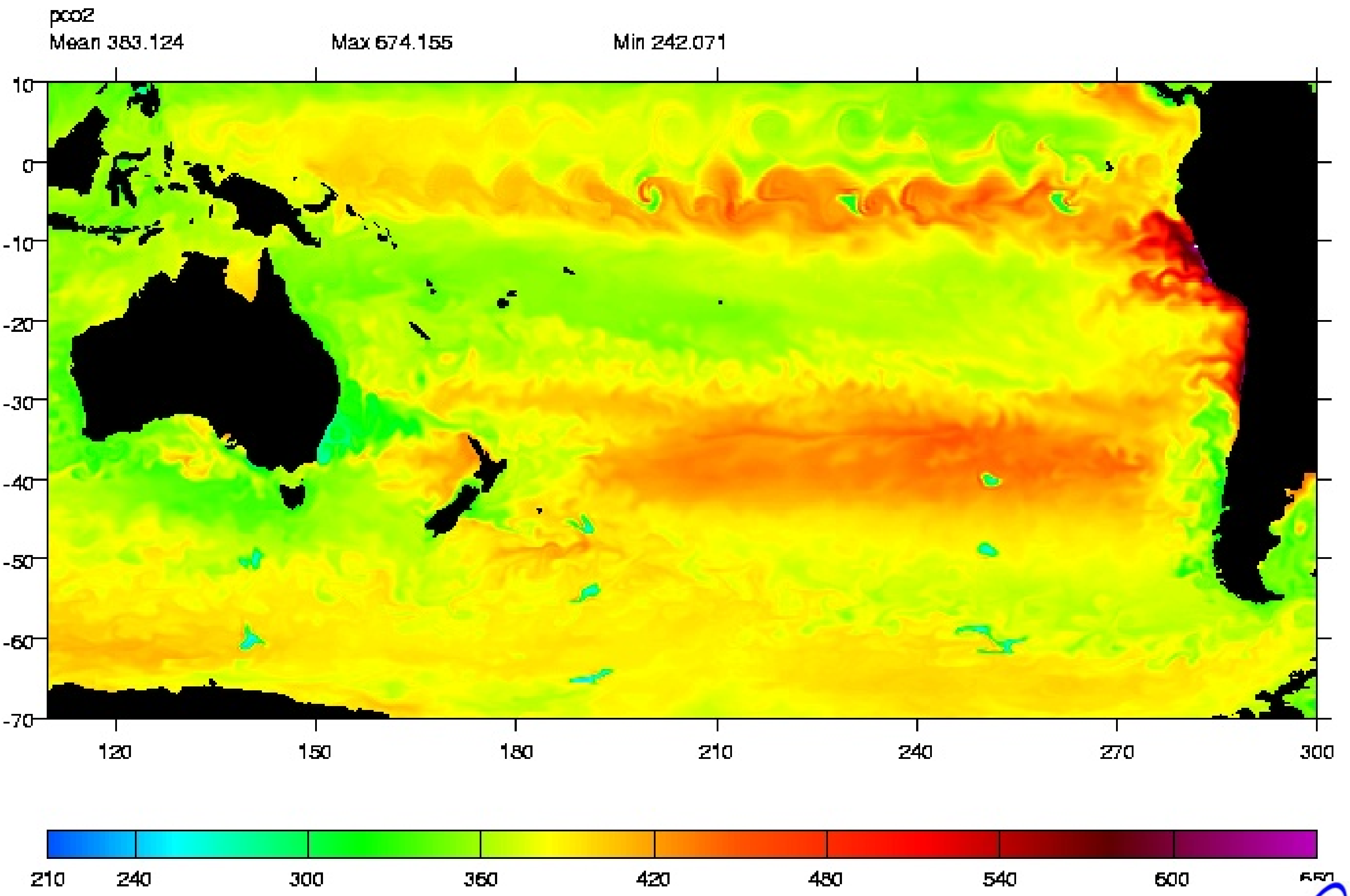
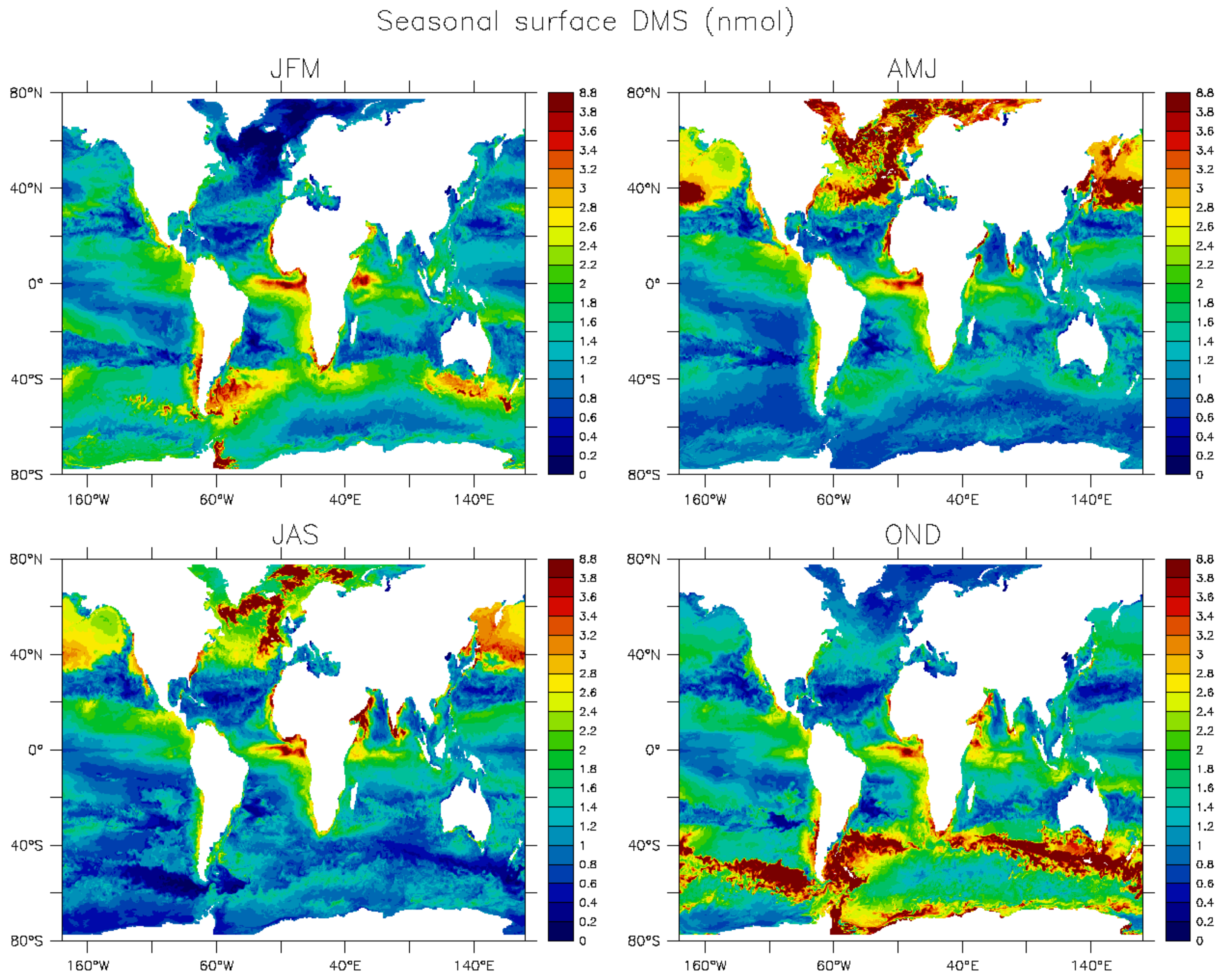
Phytoplankton at 20 days (μM N)



pCO_2 Distribution 20 days after Fertilizations



/am/nearstore1/vol/vol2/ice-bio/spchu/1280_18tracer/bf.set/movies/patch/mfp1.11 b.19990121.nc


Seasonal surface DMS (nmol)
JFM
AMJ
JAS
OND
80°N
40°N
0°
40°S
80°S
160°W
60°W
40°E
140°E
8.8
3.8
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0

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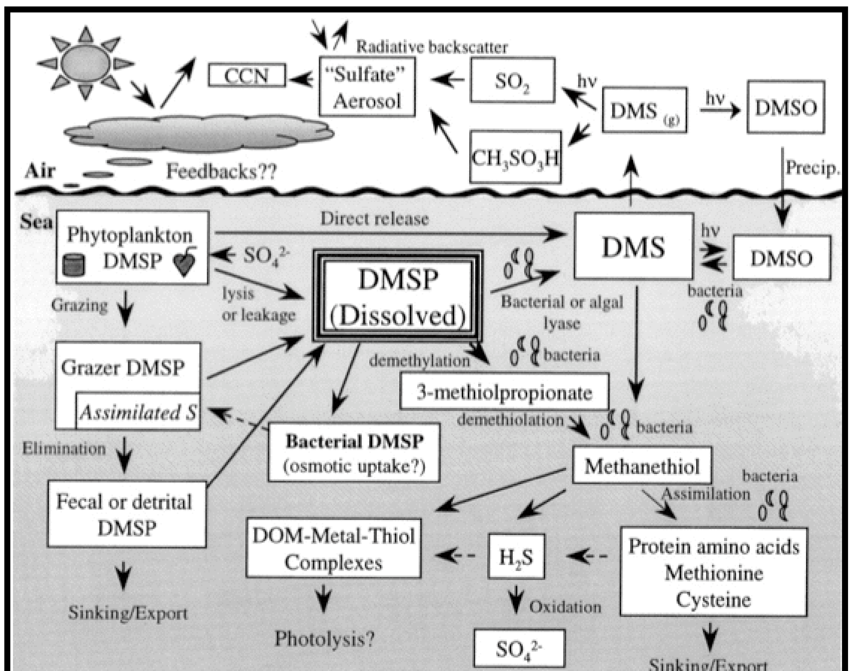
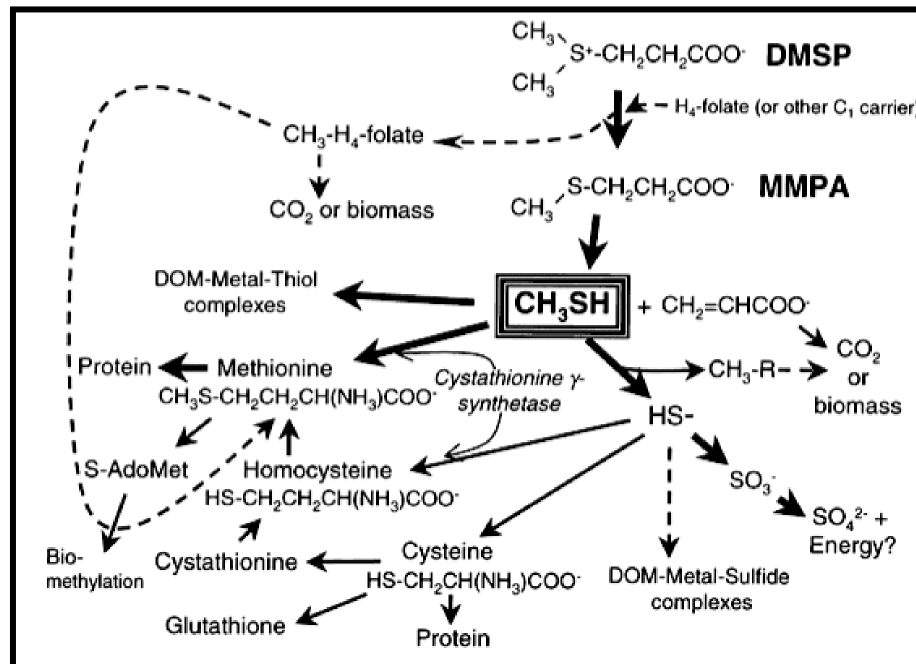
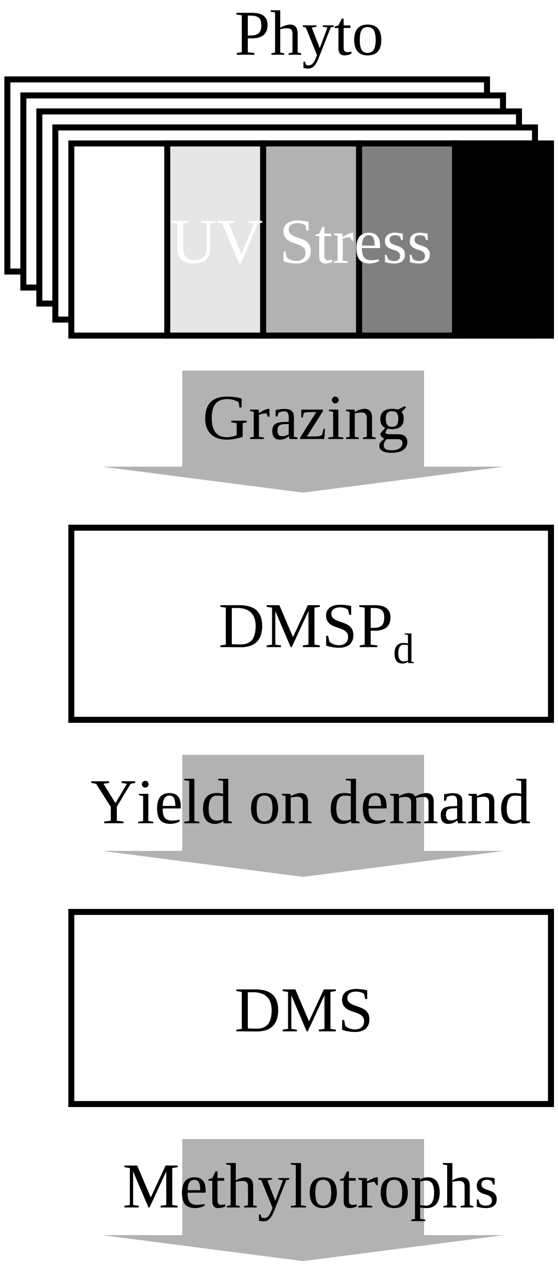




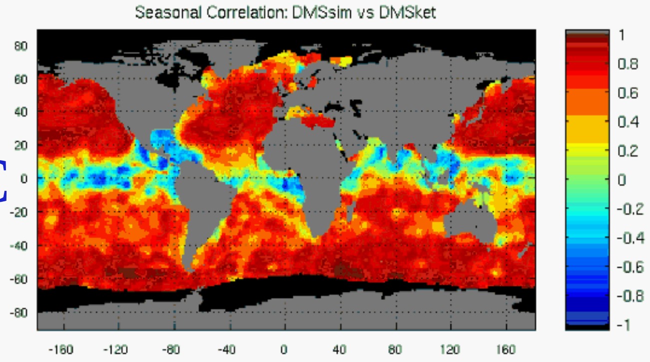


HAM (formal chi^2)	NOR (1st principles)	LANL (fuzzy steps)
	f(z)	$Dose_s$
Modular	Online	Modular
Tracer	Tracer	Split
		f(T)
Tracer	Tracer	Tracer
	Diagnose	Diagnose

DMSmodel vs DMSkettle

Statistical

BARC

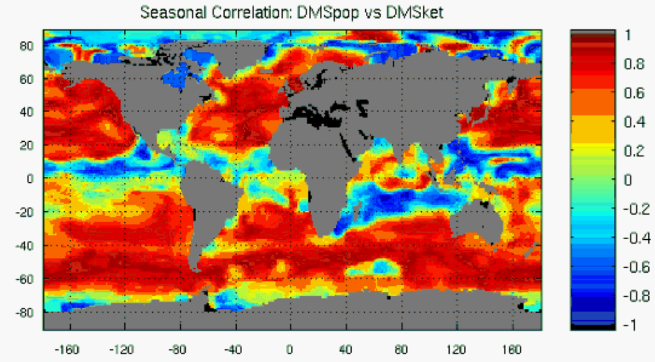


PAR

HAD

Dynamic

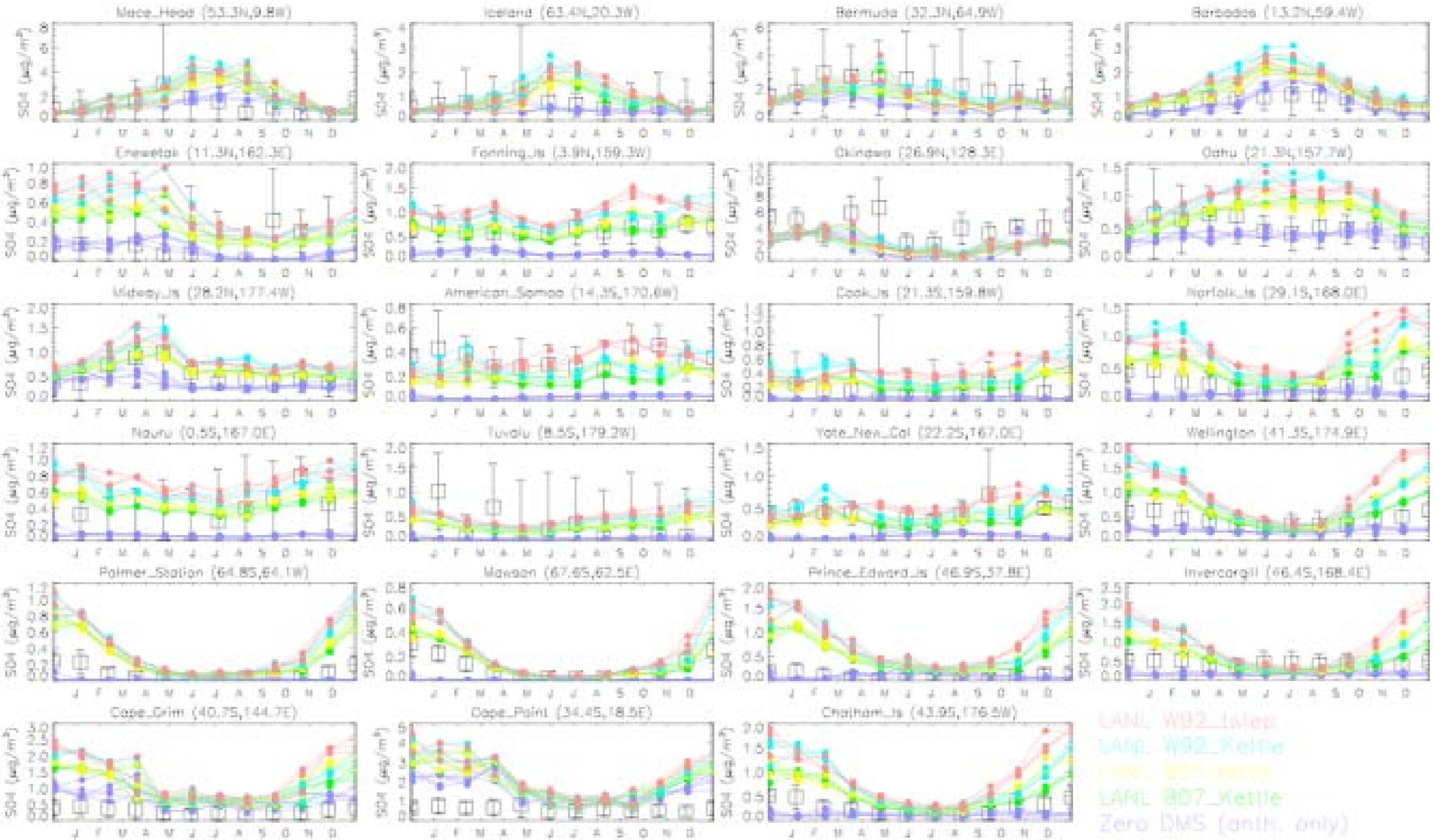
LANL



NOR

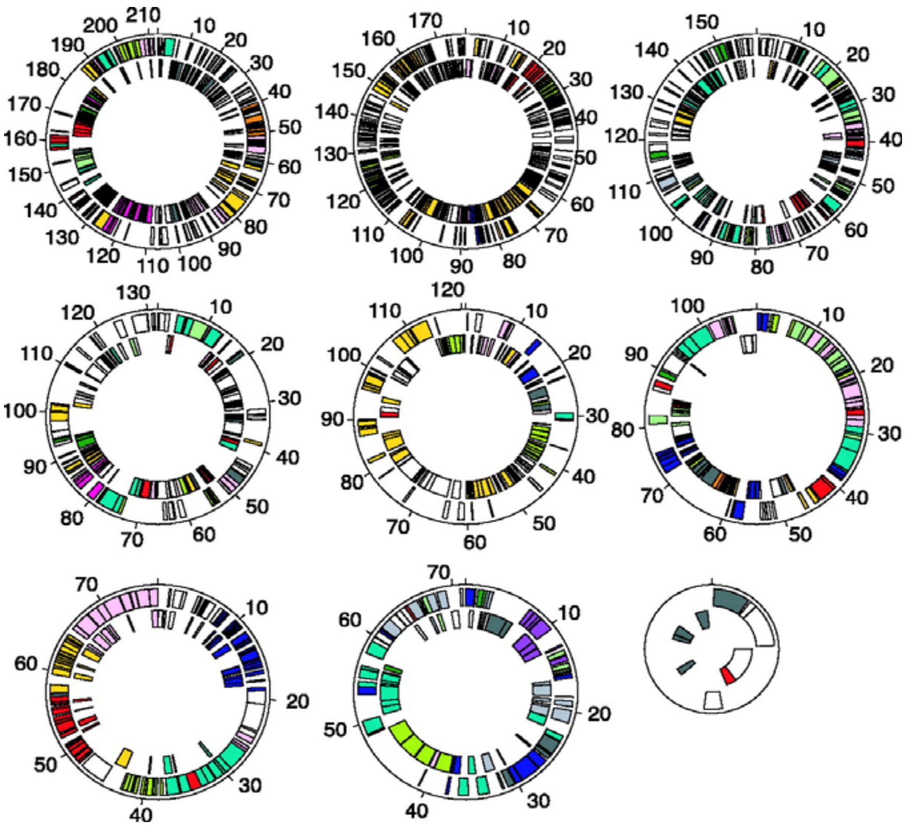
HAM

Aerosol Sulfate from DMS Fluxes, Off Line in CAM



Gene Function

TIGR role category	Total genes
Amino acid biosynthesis	37,118
Biosynthesis of cofactors, prosthetic groups, and carriers	25,905
Cell envelope	27,883
Cellular processes	17,260
Central intermediary metabolism	13,639
DNA metabolism	25,346
Energy metabolism	69,718
Fatty acid and phospholipid metabolism	18,558
Mobile and extrachromosomal element functions	1,061
Protein fate	28,768
Protein synthesis	48,012
Purines, pyrimidines, nucleosides, and nucleotides	19,912
Regulatory functions	8,392
Signal transduction	4,817
Transcription	12,756
Transport and binding proteins	49,185
Unknown function	38,067
Miscellaneous	1,864
Conserved hypothetical	794,061
Total number of roles assigned	1,242,230
Total number of genes	1,214,207



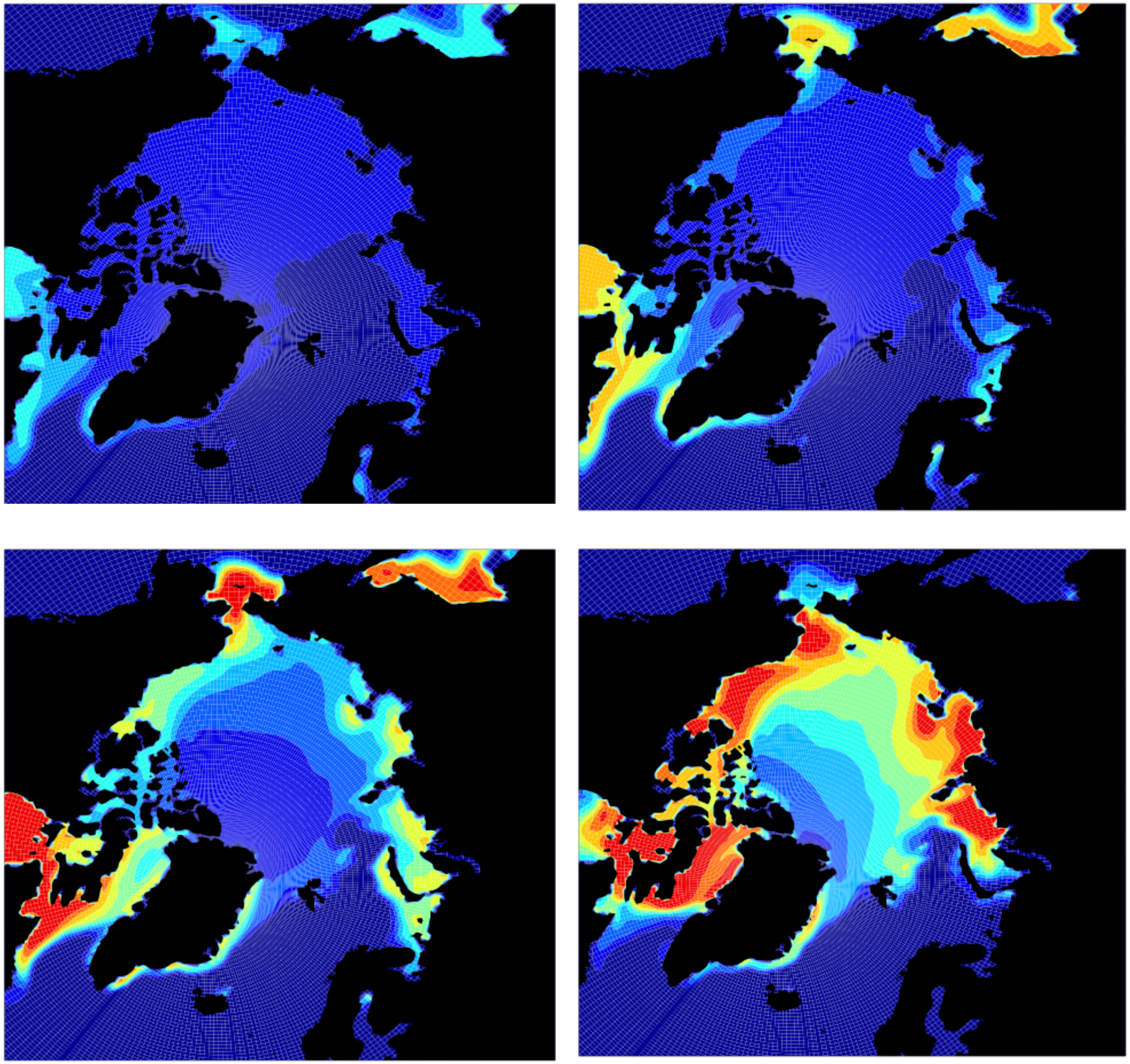
EXTRAS 2

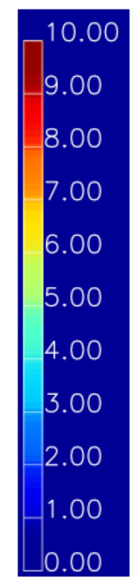
ANIMATE GROWTH

Ice Algae

Feb Mar
Apr May

Nitrogen,
Millimoles/m2

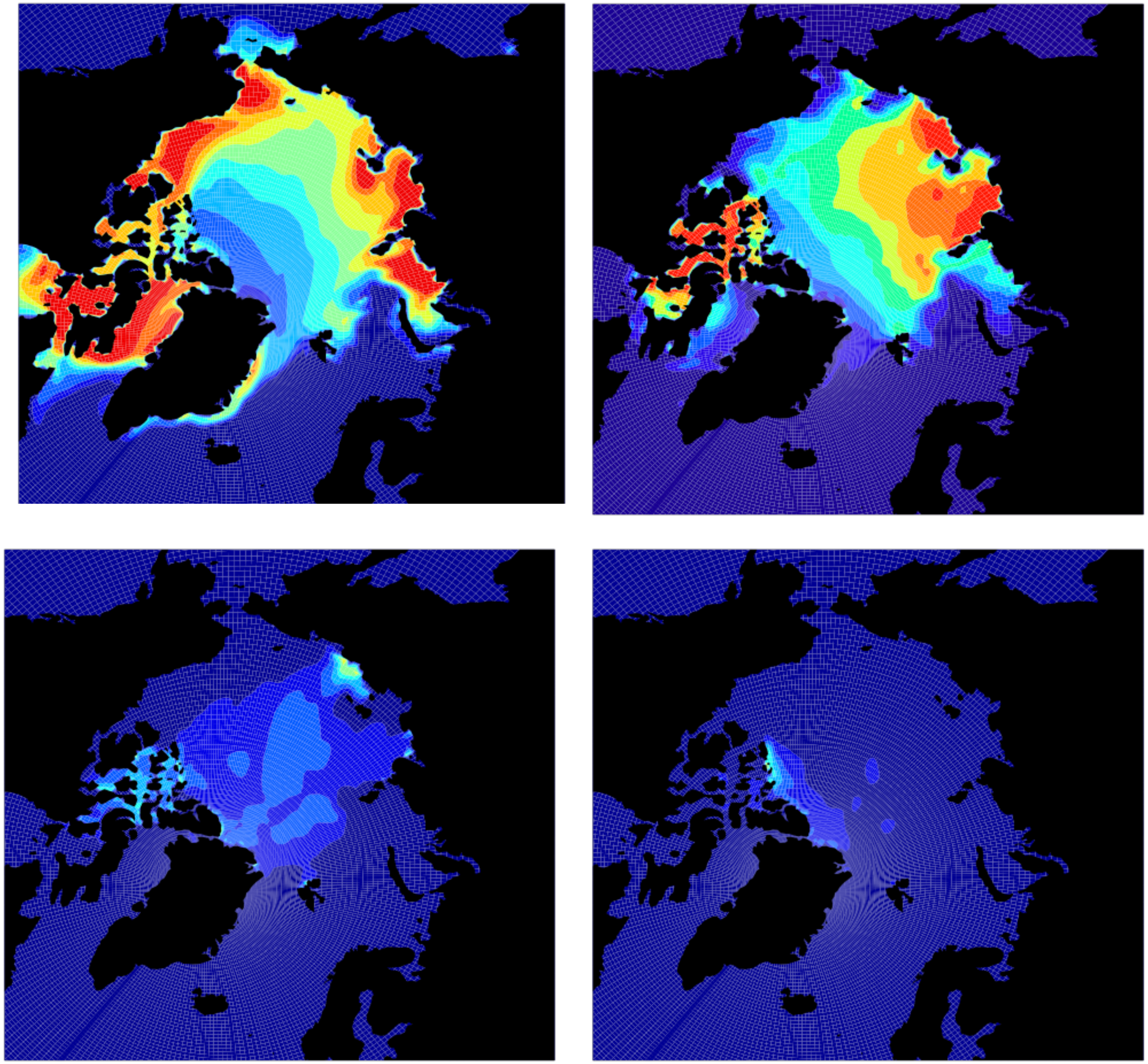


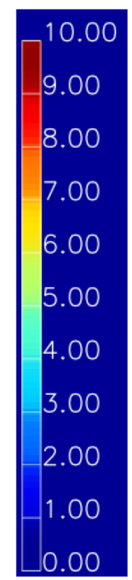


Ice Algae

May Jun
Jul Aug

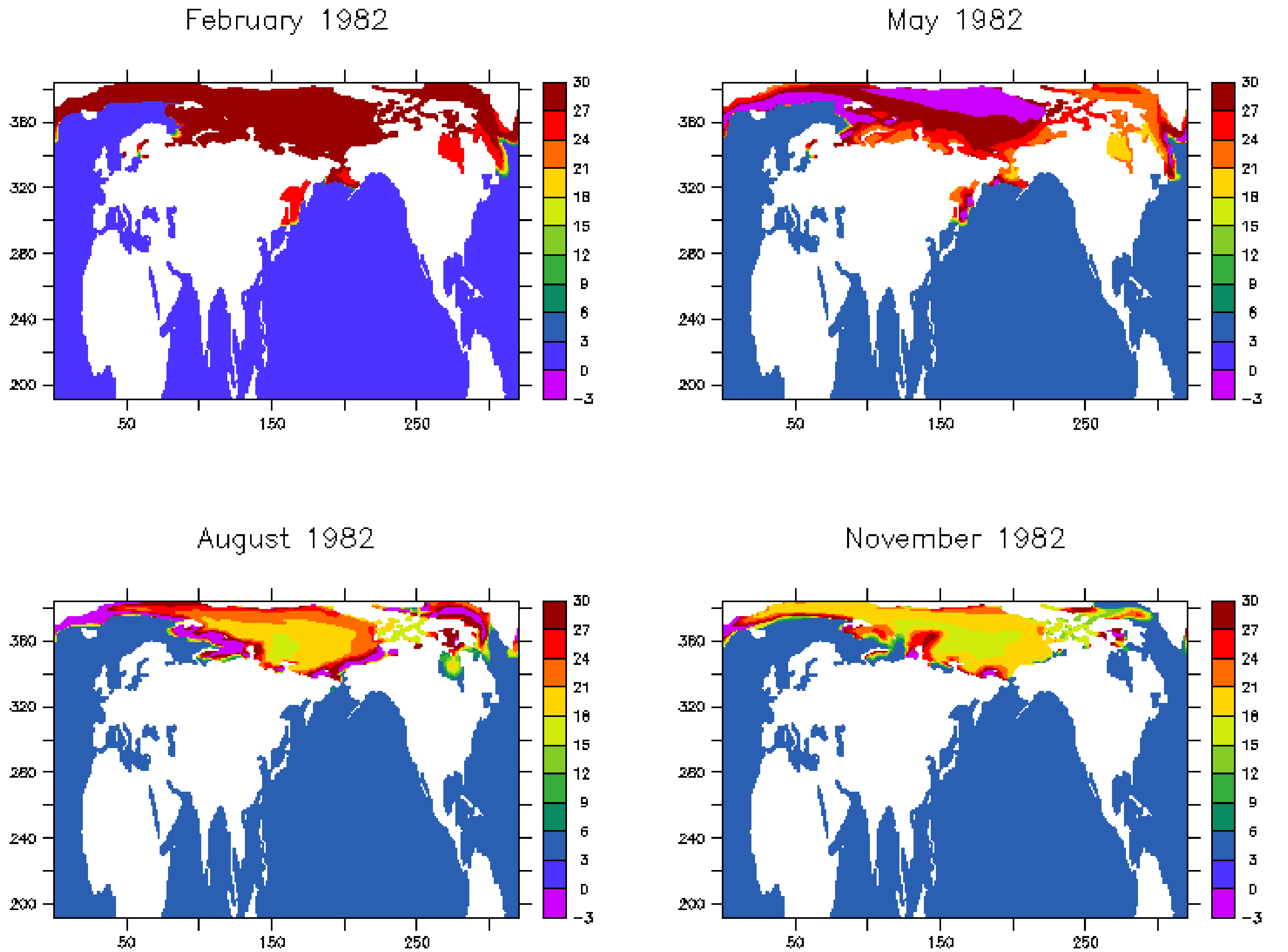
Nitrogen,
Millimoles/m2



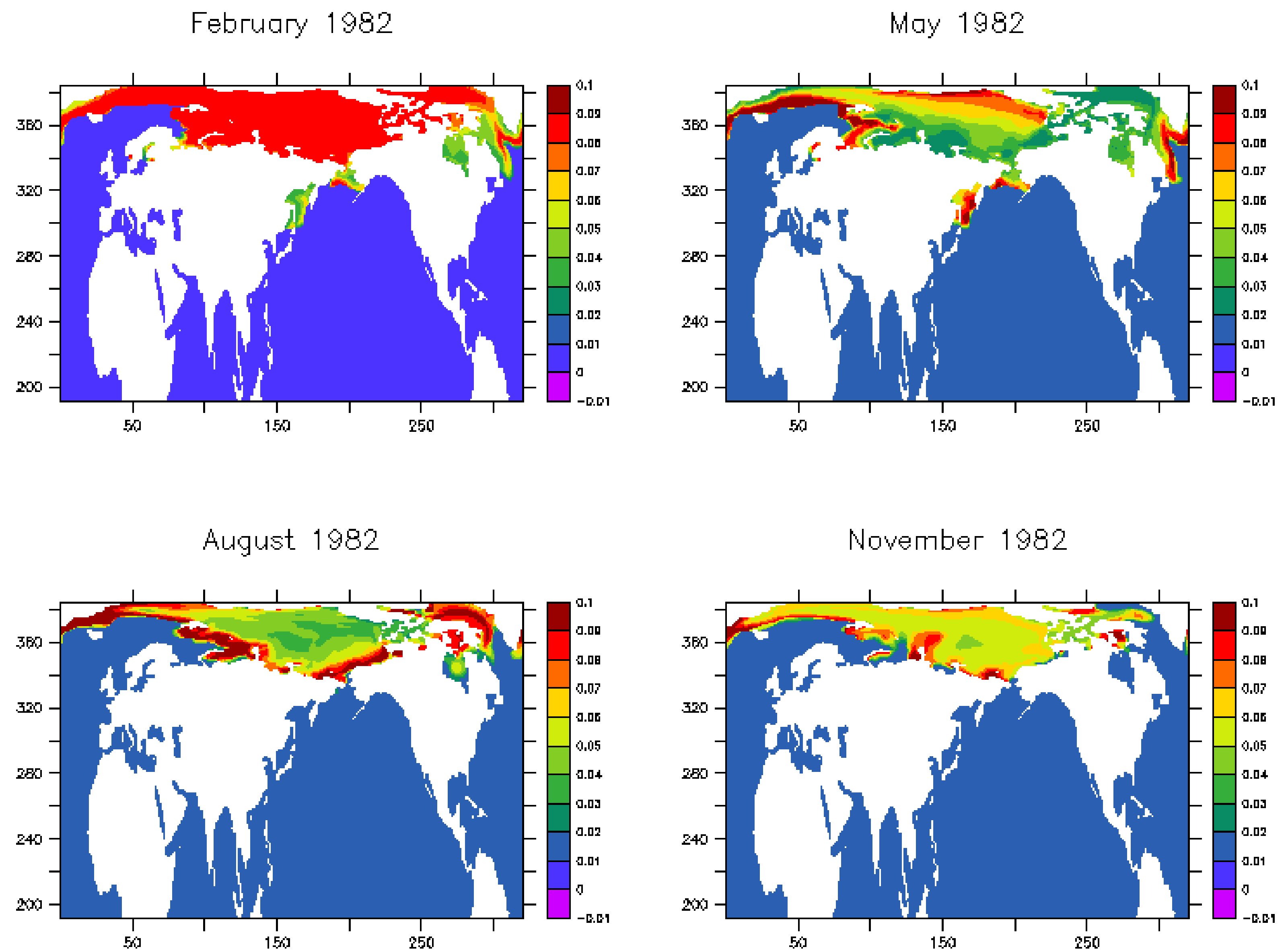


NH Si LOGICAL

Silicon in the Water Column (mmole/m2)

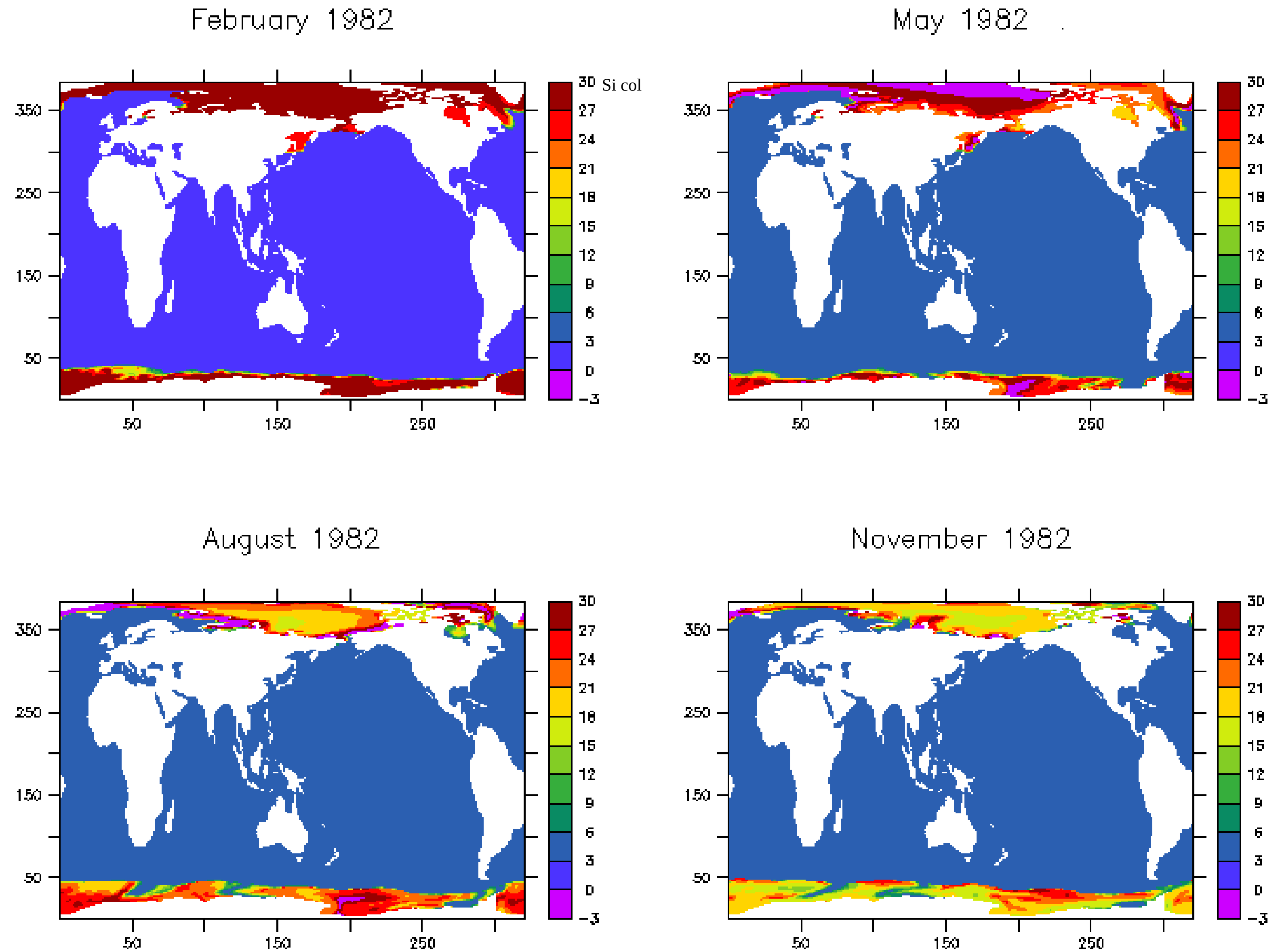


Silicon in the Skeletal Layer (mmole/m2)

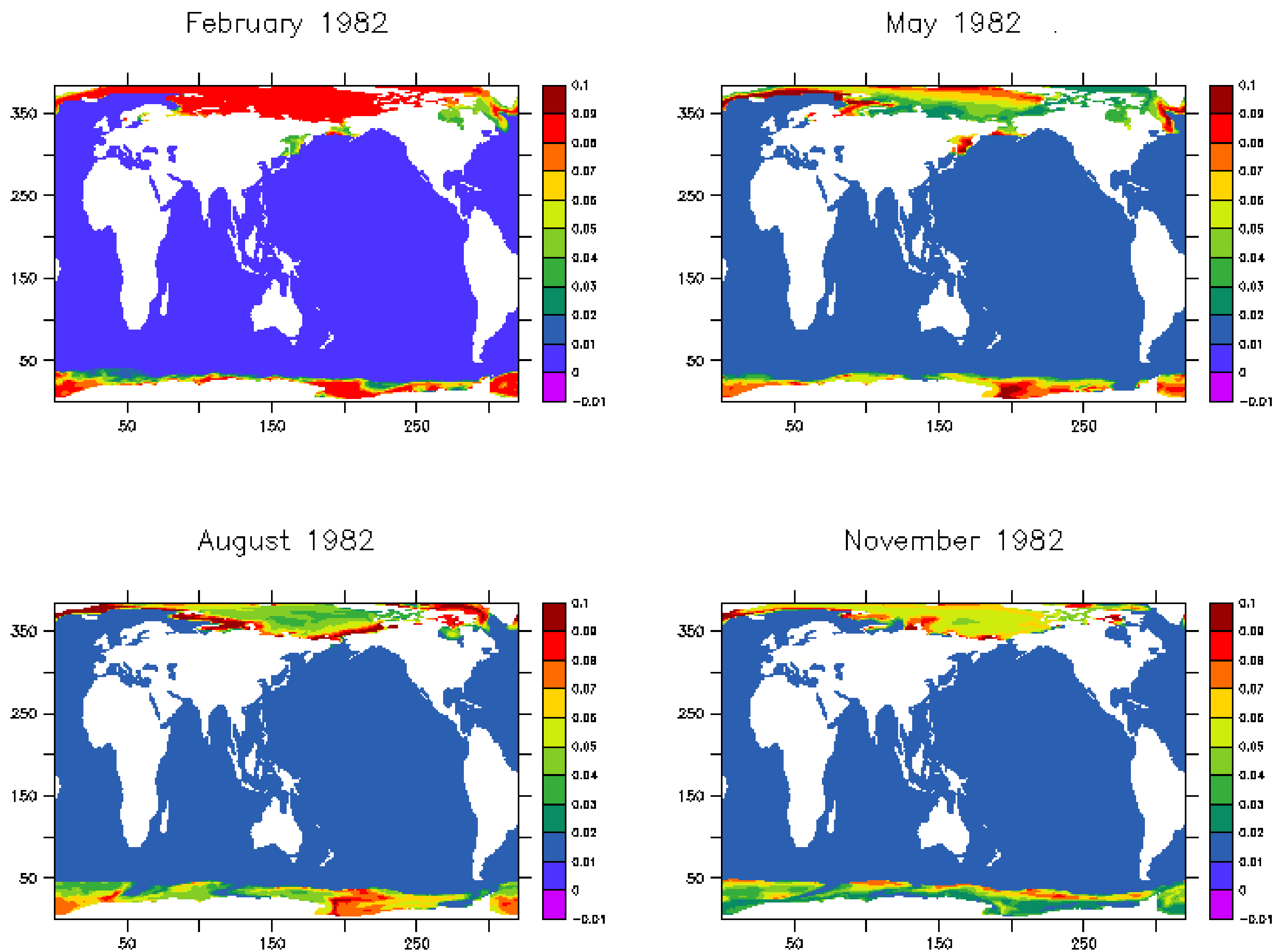


GLOBAL SI LOGICAL

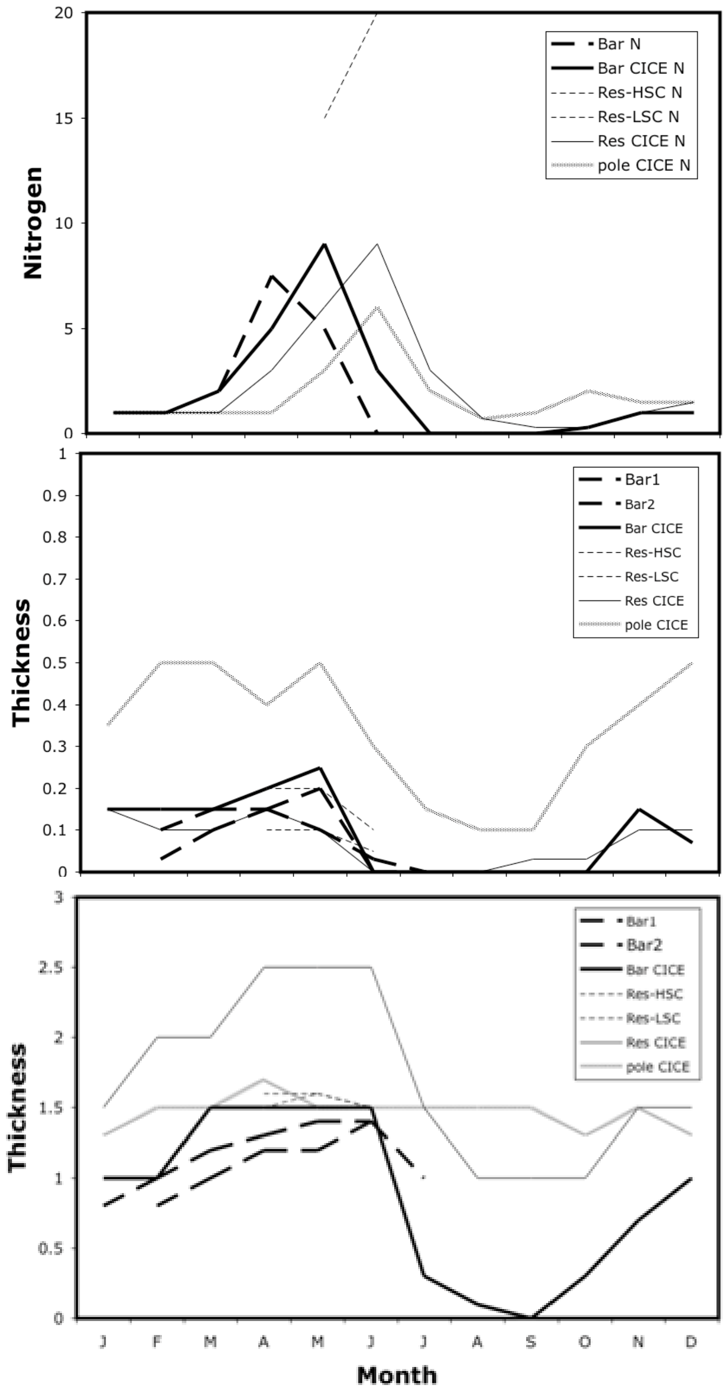
Silicon in the Water Column (mmole/m2)



Silicon in the Skeletal Layer (mmole/m2)



EXCEL Line Plots



Algal Nitrogen - mmoles/m2
Snow Thickness - m
Ice Thickness - m

Data - dashed
Model - solid

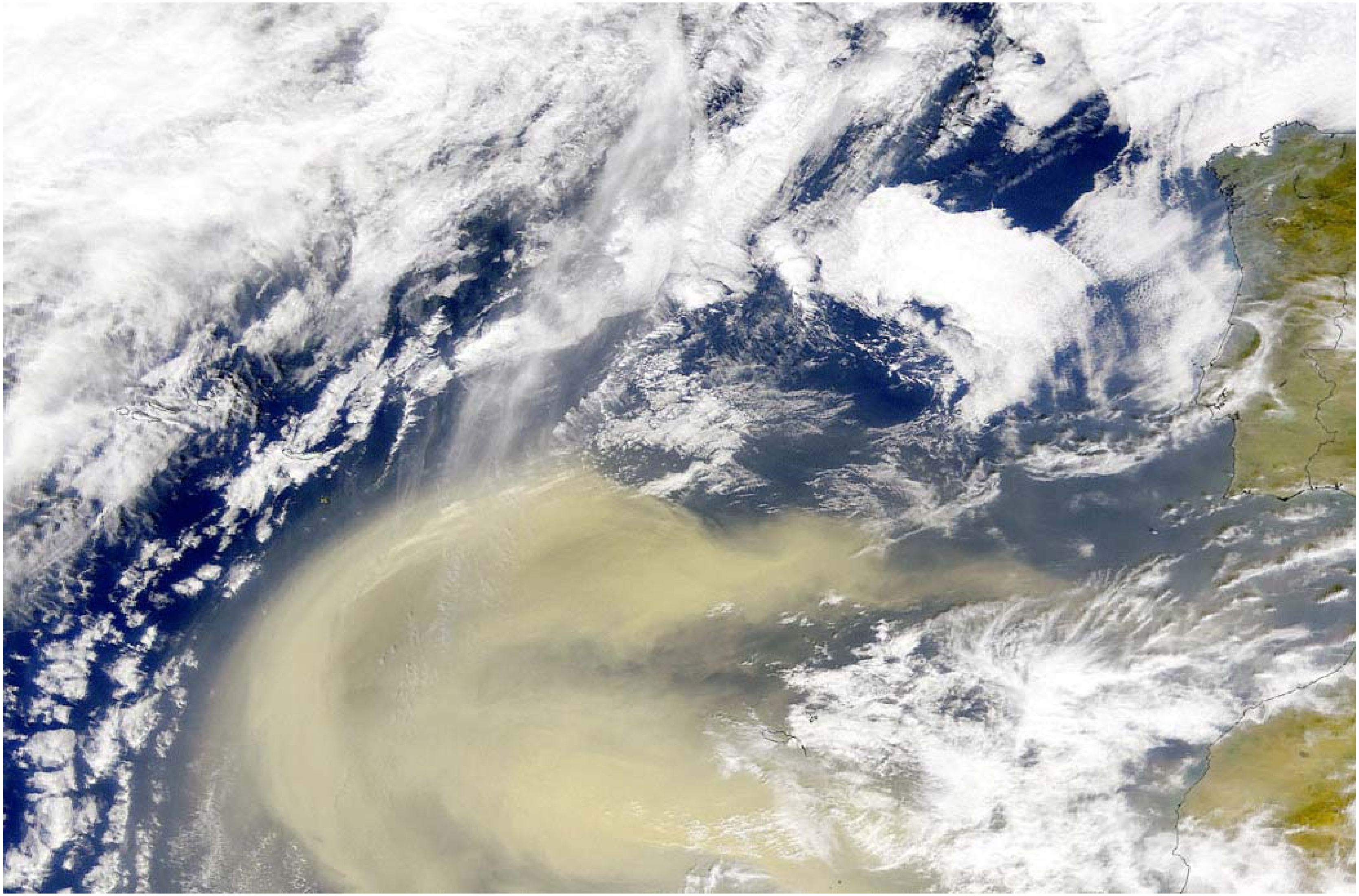
Barrow - Thick
Resolute - Thin
Pole - Grey tone

Blooms are solar initiated
Melt terminated

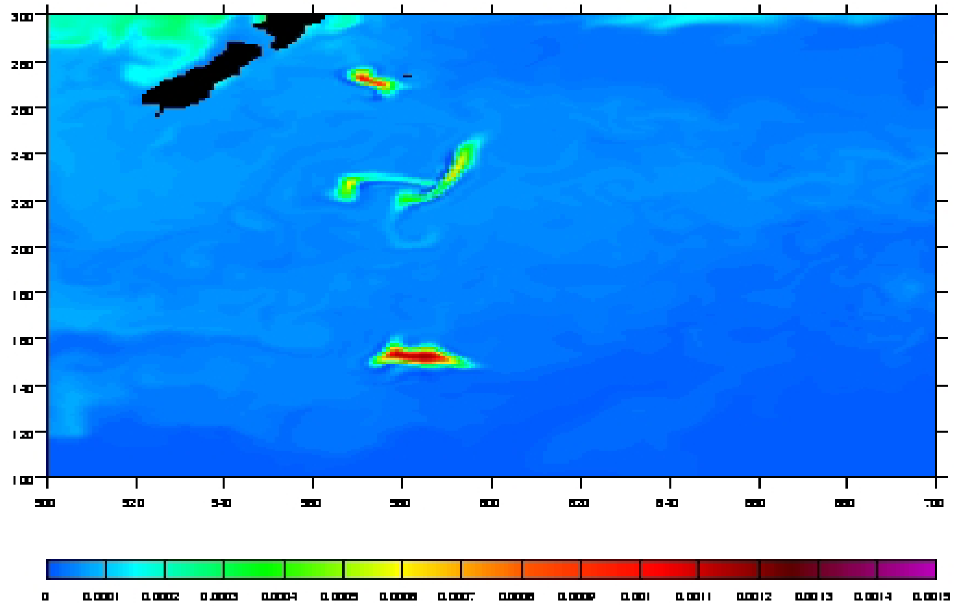
Resolute Low Snow Case
Singular - Coastal?

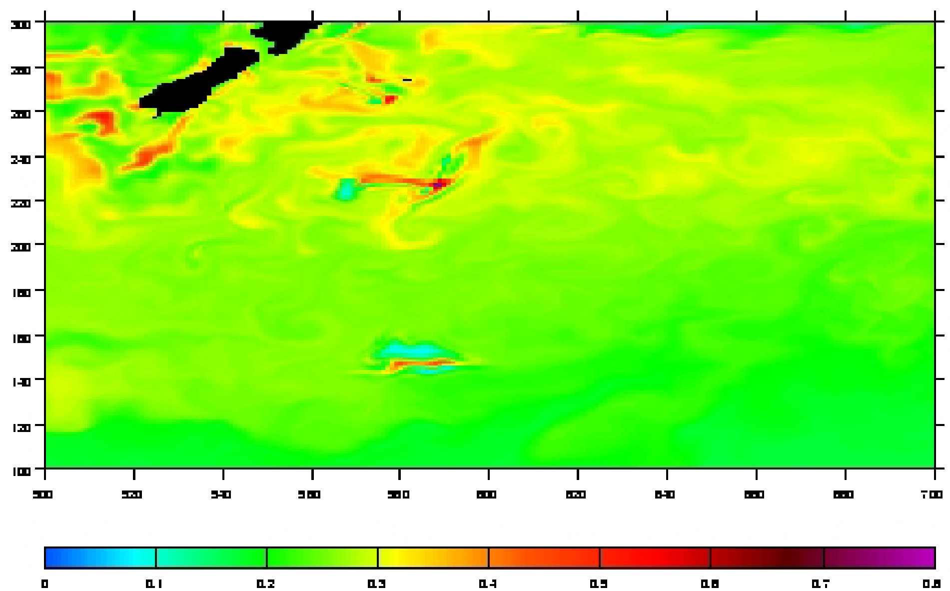
OLDER

Iron control over a quarter of the planet



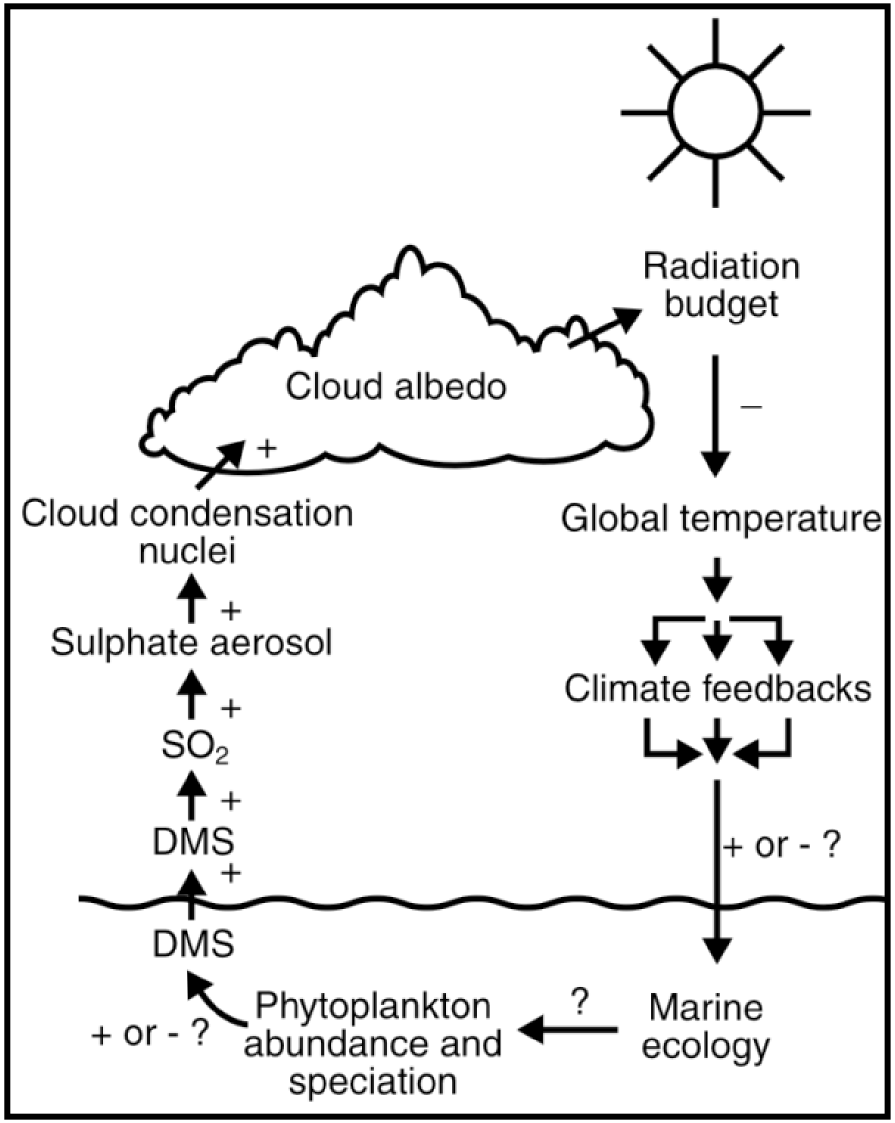
Iron and Phytoplankton in SOFeX Simulation





Los Alamos
NATIONAL LABORATORY

MOTIVATION



- **Community driver continues to be CLAW**
- **Ours is to use SciDAC machinery to help quantify**
- **Magnitude, sign of ecosystem effects remain uncertain**
- **Only detailed modeling can alleviate the situation**
- **That's us, so our life is now sulfur**

Charlson et al. 1987

Prochlorococcus gene conservation