The Transport Matrix Method (TMM)
(for fast, offline simulation of passive tracers in the ocean)

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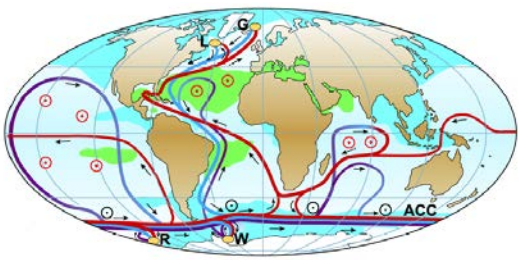
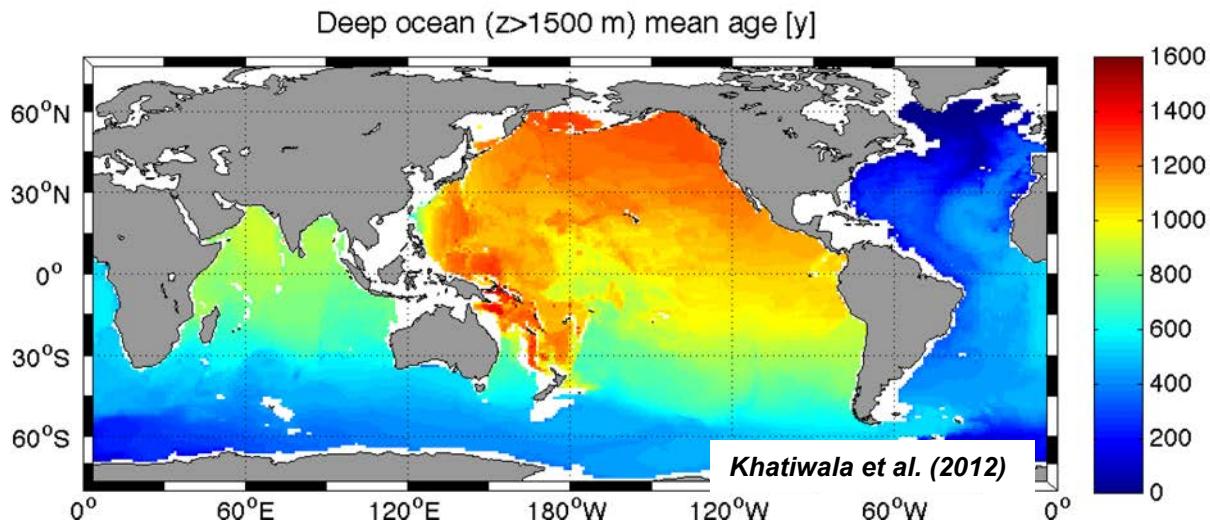
Why do we need alternatives to GCMs?

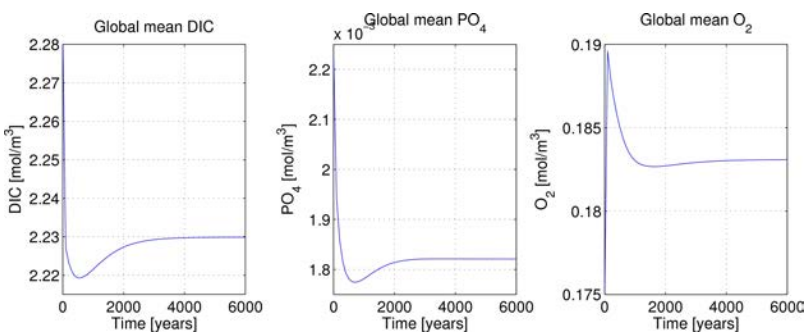
- **Ocean circulation is sluggish and highly diffusive, and the time scale for ocean transport is O(1000s) of years …**



Kuhlbrodt et al, 2007



Deep ocean (>1500 m) mean age computed using inverse estimate of ocean Green's function



- **… 4000-5000 y-long integrations are required for biogeochemical and proxy tracers to equilibrate:**
- **y = H(x) is very expensive!**

A matrix approach to tracer transport

Continuum tracer advection-diffusion equation:

$$\frac{\partial c}{\partial t} = -\nabla \cdot (\mathbf{u}c) + \nabla \cdot \kappa \nabla c + \mathrm{SGS}(c) + q(c,t)$$

Discrete time-stepping equation for a **passive** tracer can be written in matrix form:

$$\mathbf{c}^{n+1} = \mathbf{A}^n \mathbf{c}^n + \mathbf{q}^n$$

- **c** is the vector of tracer concentrations
- *n* is the time step
- **A** is the "transport matrix" (includes the effects of advection, diffusion, and (parameterized) SGS processes)
- **q** is the source/sink term for the tracer

Khatiwala et al. (2005)*; *Khatiwala (2007)

Any discretized linear tracer equation can be written in matrix form

A 1-d example

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2} \qquad 0 < x < L,$$

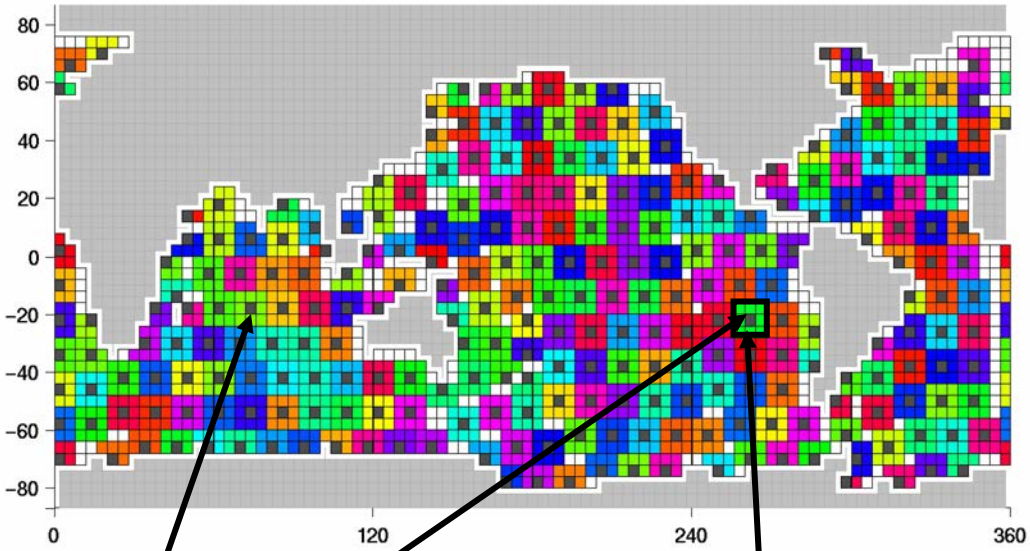
$$c(x=0,t) = a(t) \text{ and } c(x=L,t) = b(t)$$

$$c_i^{n+1} = c_i^n + \frac{\kappa \Delta t}{(\Delta x)^2}(c_{i+1}^n - 2c_i^n + c_{i-1}^n), \quad i = 1, \ldots, M$$

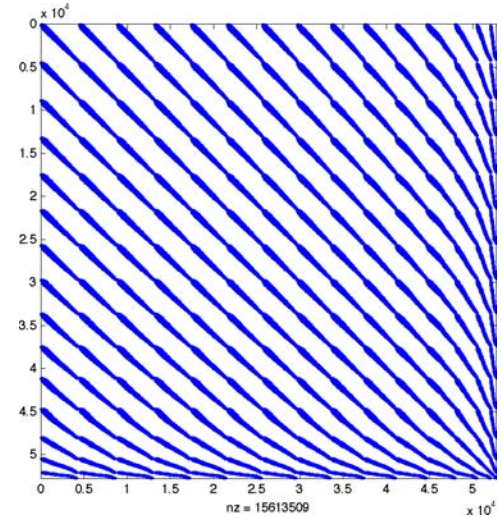
$$c_0^n = a(n\Delta t) \text{ and } c_{M+1}^n = b(n\Delta t)$$

$$\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{M-1} \\ c_M \end{bmatrix}^{n+1} = \begin{bmatrix} 1-2\alpha & \alpha & & & & \\ \alpha & 1-2\alpha & \alpha & & & \\ & & \ddots & & & \\ & & & \alpha & 1-2\alpha & \alpha \\ & & & & \alpha & 1-2\alpha \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_{M-1} \\ c_M \end{bmatrix}^n + \begin{bmatrix} \alpha & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ 0 & \alpha \end{bmatrix} \begin{bmatrix} c_0 \\ c_{M+1} \end{bmatrix}^n, \quad \alpha = \frac{\kappa \Delta t}{(\Delta x)^2}$$

We can *empirically* construct A for any GCM by "probing" it with a passive tracer



Typical sparsity pattern of A



Grid points where δ's are applied

In *one* time-step influence of δ only felt in a limited "halo" around grid point

Use graph coloring to identify "structurally independent" columns of A and compute a large number of columns *simultaneously*

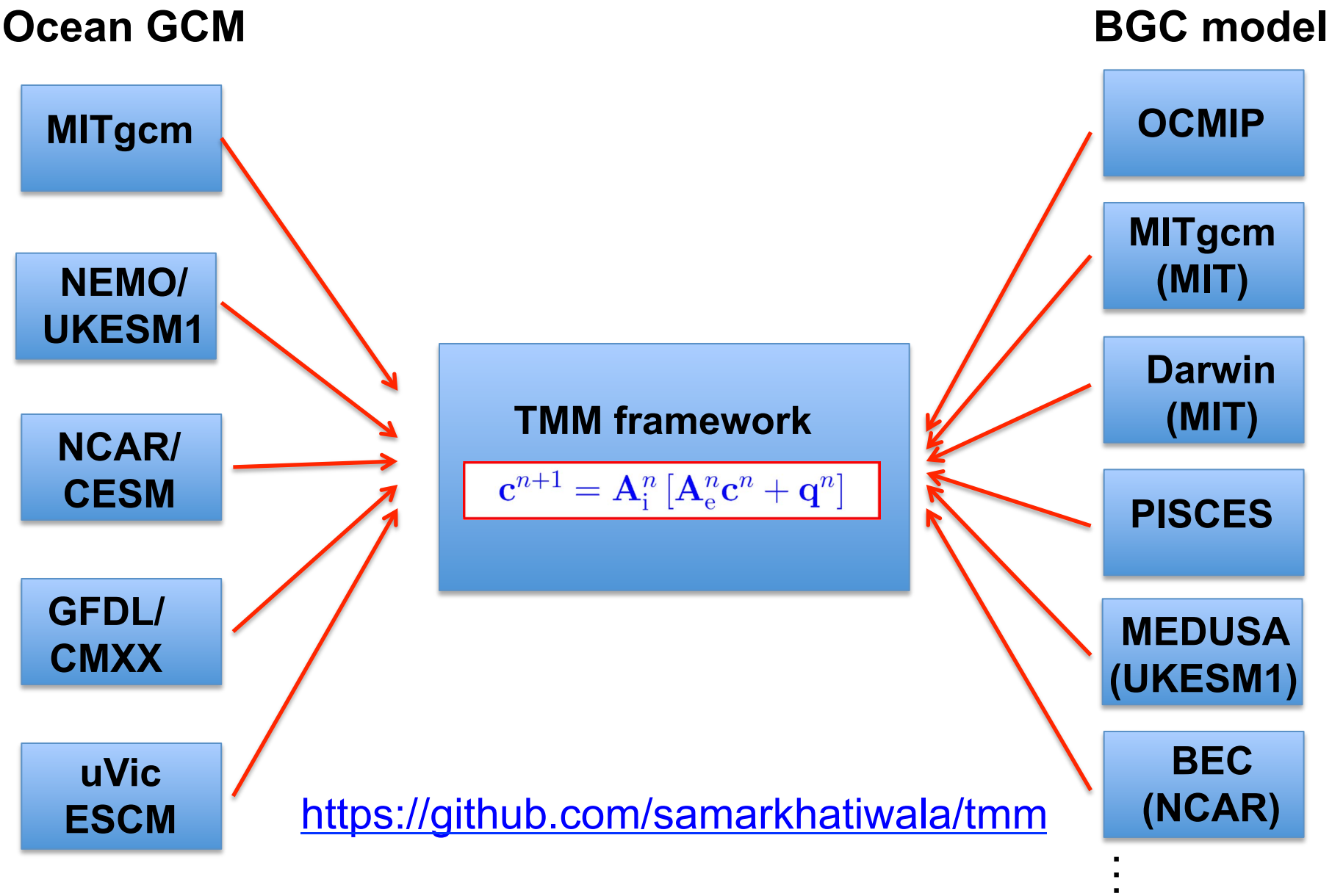
What good is all this?

- Circulation embedded in the TMs accurately represents the complex 3-d advective-diffusive transport (including all sub-grid scale parameterizations) of the underlying GCM.
- Once the TMs are known, the GCM can be dispensed with: tracer transport is simple a sequence of **sparse** matrix-vector products. We know how to do this very efficiently on parallel machines.

$$\mathbf{c}^{n+1} = \mathbf{A}_{\mathrm{i}}^{n}\left[\mathbf{A}_{\mathrm{e}}^{n}\mathbf{c}^{n} + \mathbf{q}^{n}\right]$$

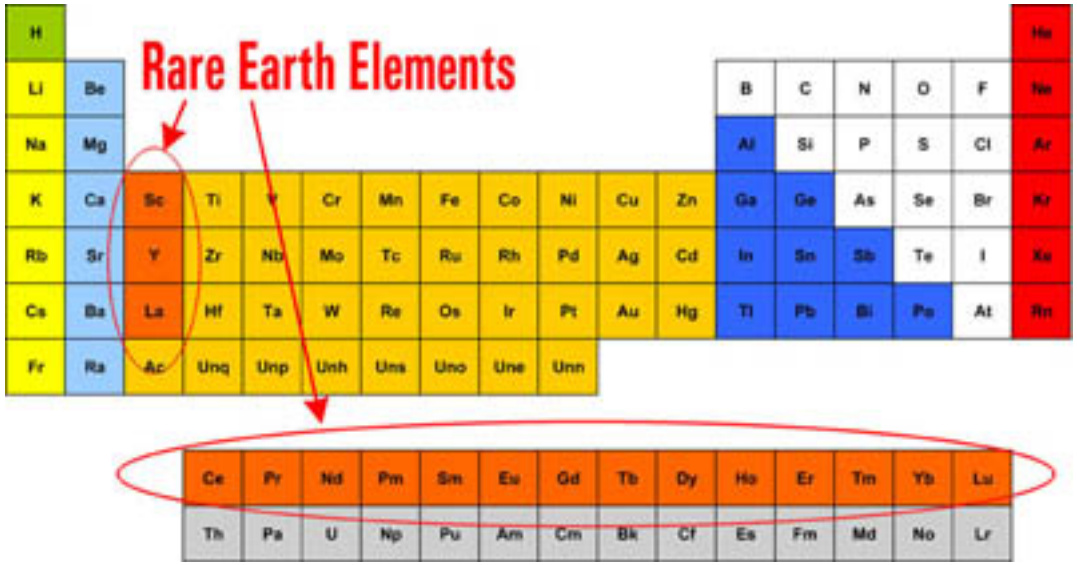
e.g., MITgcm ECCO-v4 ¼º, 50 levels: N=2.5x10^6, nnz($\mathbf{A}_e$)=0.0011%

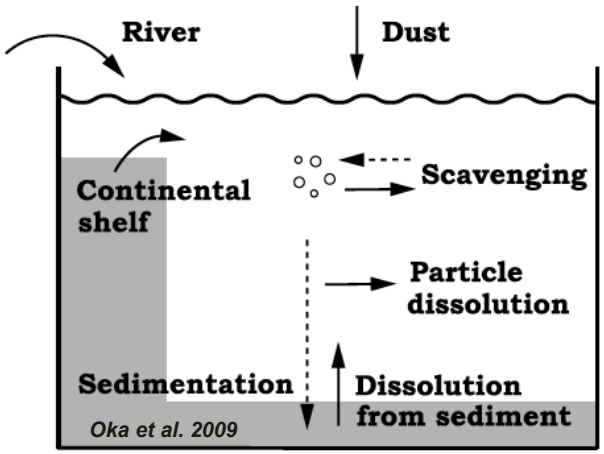
Biogeochemical model (q) is "decoupled" from the tracer transport: one can mix and match ocean circulation and biogeochemical models



https://github.com/samarkhatiwala/tmm

Modeling Rare Earth Elements (REEs)

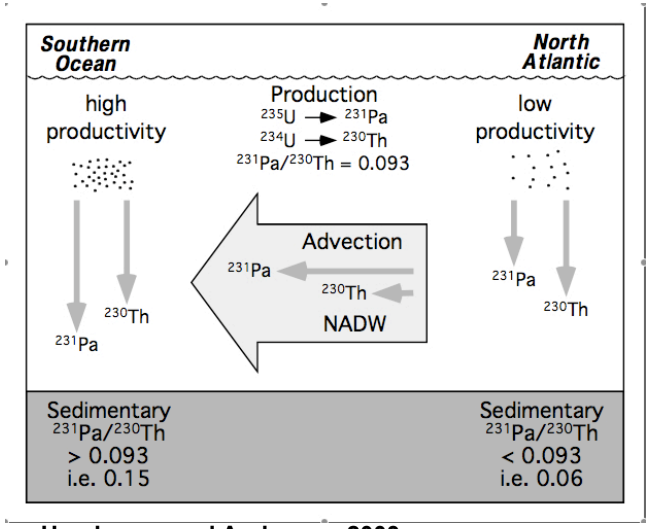




- REEs are a coherent sequence of purely scavenged tracers.
- They are also a tool to elucidate the role of scavenging of other trace elements such as Fe and Zn.
- Nd isotopes for example are used as a proxy of past ocean circulation and climate.
- Ce is used as a paleo-proxy of redox conditions.
- Additionally, Pa and Th have long been used as proxies for ocean circulation and flux of biogenic particles.

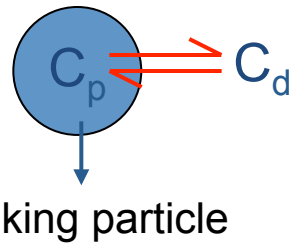
Yves Plancherel, Oxford

Example: ^{231}Pa and ^{230}Th with reversible scavenging



Henderson and Anderson, 2003

Reversible scavenging $K = \dfrac{\{REEParticle\}}{\{REE^{3+}_{free}\} \cdot \{Particles\}}$



$$\frac{\partial}{\partial z}\left(w_s \frac{\sum_i K^i C^i_{\text{bulk}}(x,y,z)}{\sum_i K^i C^i_{\text{bulk}}(x,y,z)+1} C\right)$$

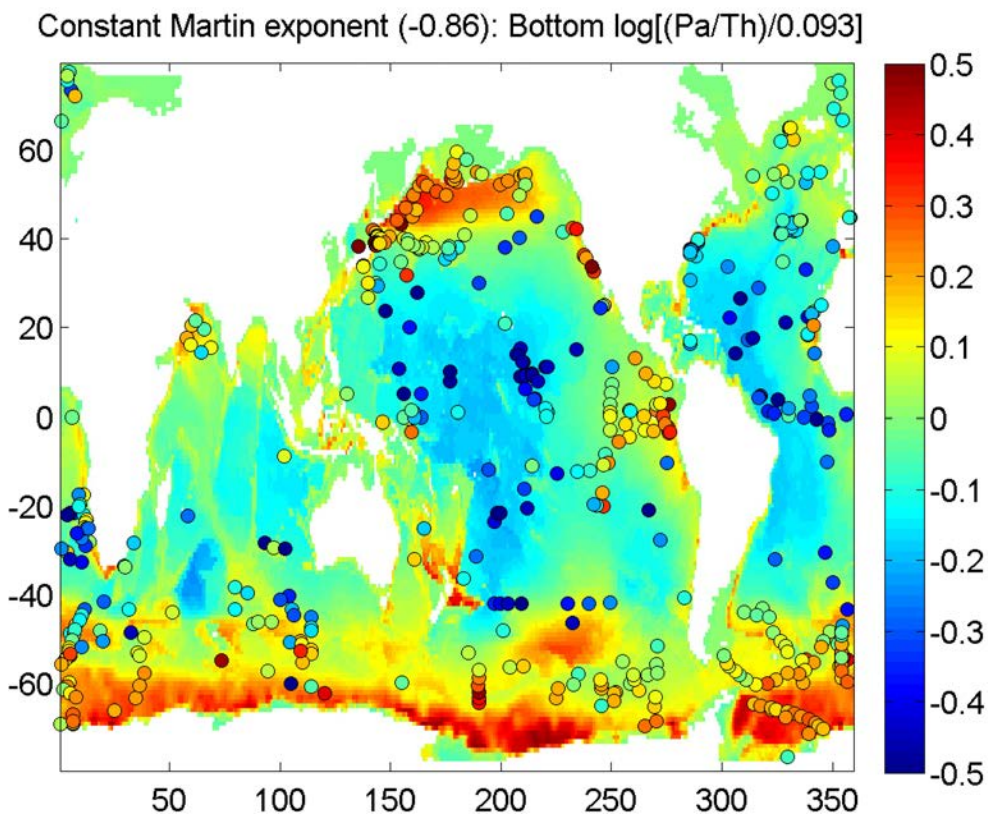
$$\mathbf{q} = -\Lambda \mathbf{c} + \beta + \mathbf{Q}_{\text{rev}} \mathbf{c}$$

If we can neglect the seasonal cycle (annual mean TM), the steady state solution satisfies a linear system of equations:

$$\left[\mathbf{A}_{\text{i}}\mathbf{A}_{\text{e}} - \mathbf{A}_{\text{i}}\mathbf{\Lambda} + \mathbf{A}_{\text{i}}\mathbf{Q}_{\text{rev}} - \mathbf{I}\right]\mathbf{c} = -\beta$$

^{231}Pa and ^{230}Th with reversible scavenging

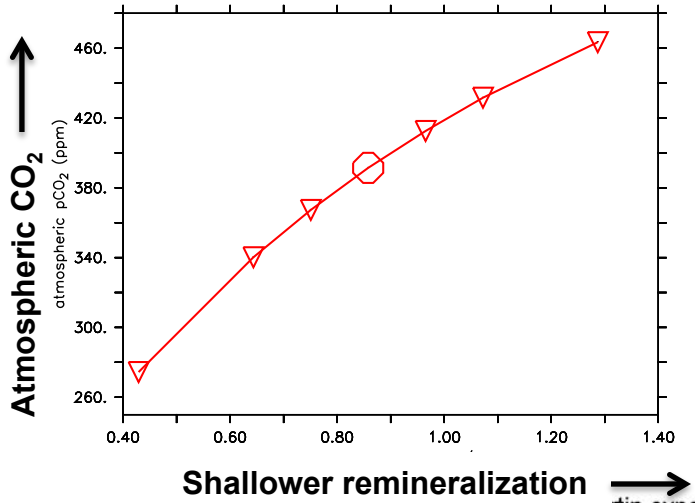
Bottom layer ^{231}Pa/^{230}Th ratio computed with TM from ECCO state estimate (1º/23 levels)

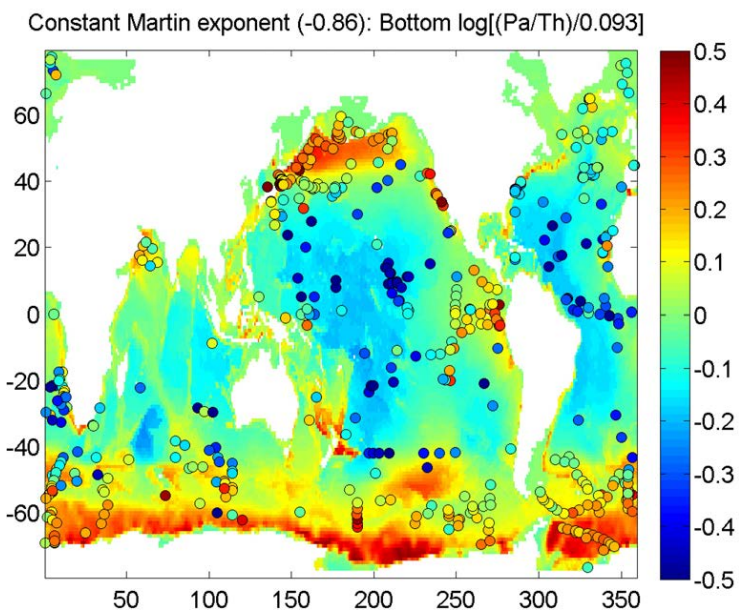


log[(Pa/Th)/0.093]

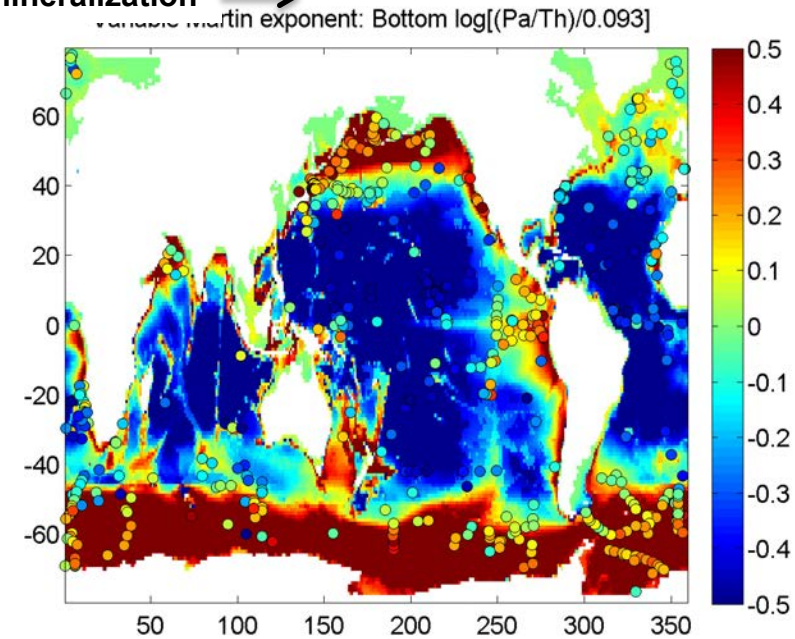
Particle flux (POC, $CaCO_3$, dust, opal) and K^i from *Siddall et al*, 2005

^{231}Pa and ^{230}Th are not only on a proxy for ocean circulation but also for ocean biogeochemistry





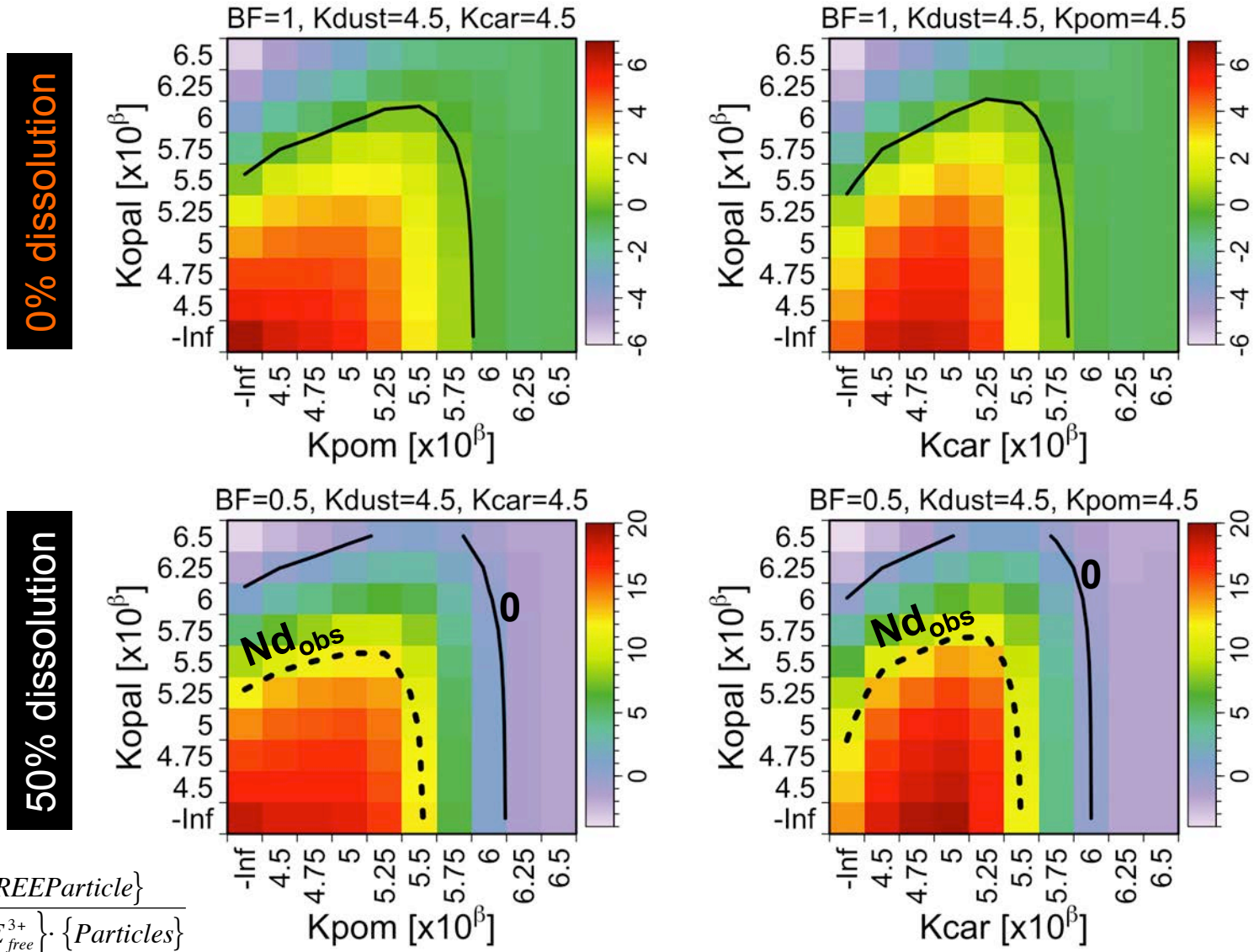
Uniform remineralization depth



Variable remineralization depth

TMM is especially useful for parameter sensitivity

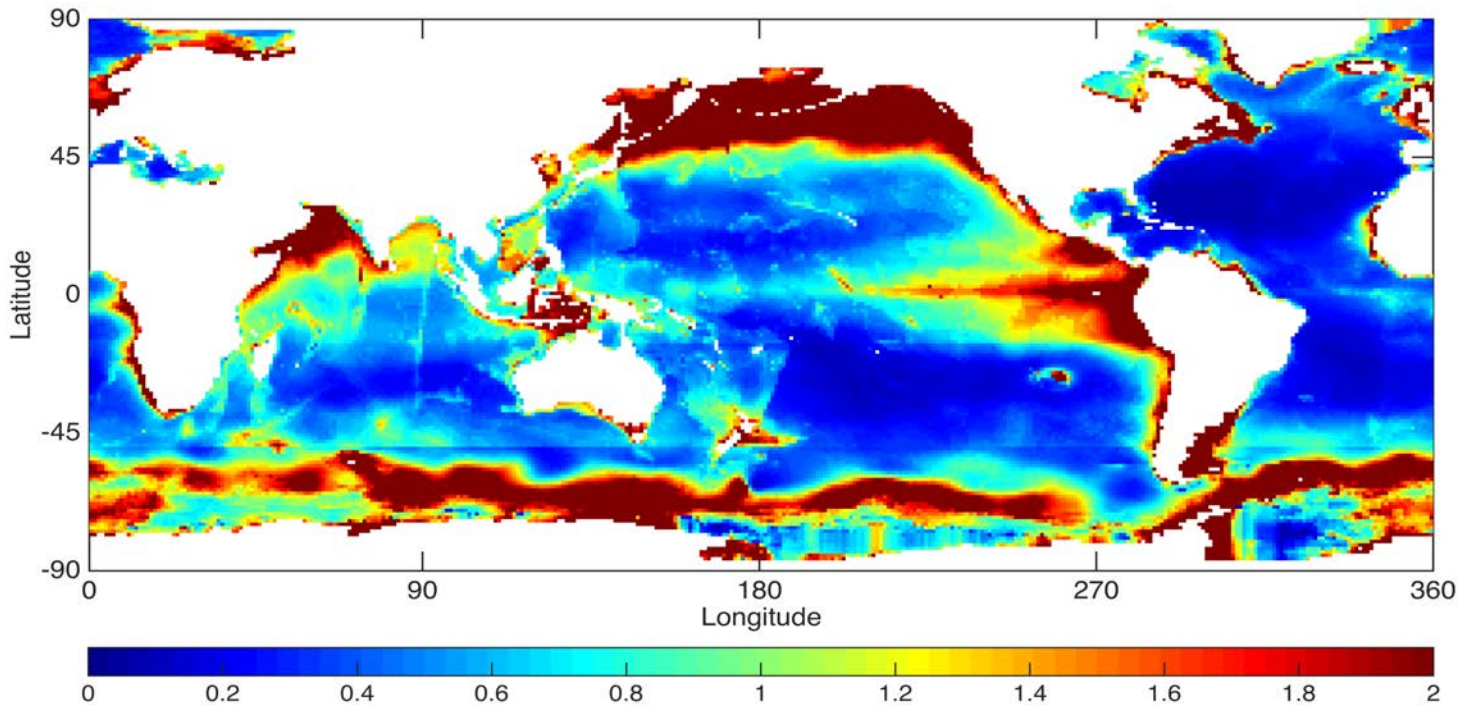
Mean deep North Pacific to North Atlantic gradient in ε_{Nd}



$$K = \frac{\{REEParticle\}}{\{REE^{3+}_{free}\} \cdot \{Particles\}}$$

Yves Plancherel, Oxford

^{10}Be proxy for solar magnetic field & irradiance: where is the best place in the ocean to sample this tracer?



^{10}Be flux to sediments/atmospheric ^{10}Be production rate

1=optimal

Lewis Carney, Oxford

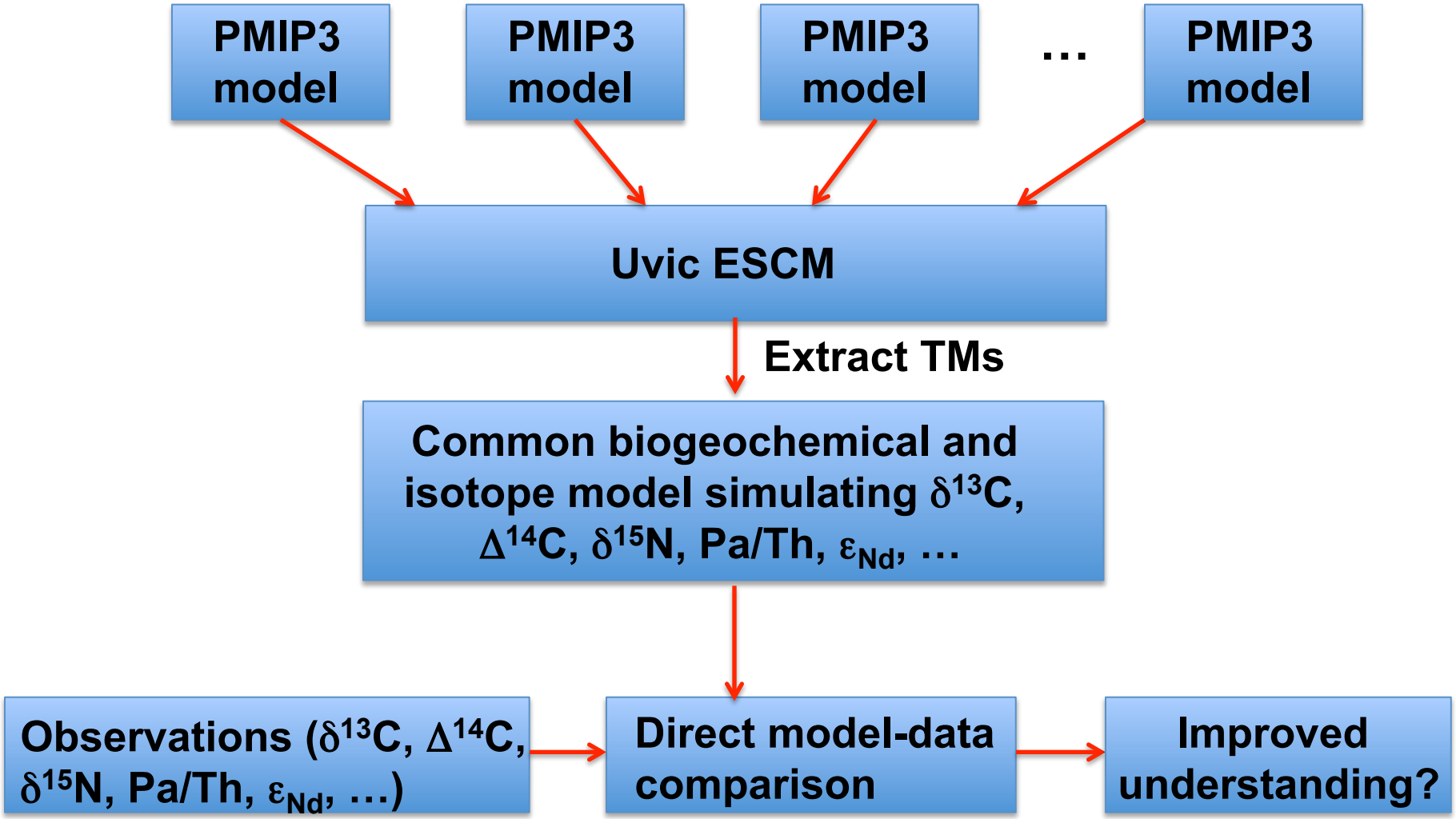
In the most general case we can simply time-step the matrix equations forward in time:

$$\mathbf{c}^{n+1} = \mathbf{A}_{\mathrm{i}}^{n}\left[\mathbf{A}_{\mathrm{e}}^{n}\mathbf{c}^{n} + \mathbf{q}^{n}\right]$$

- All this requires is the ability to perform a sparse matrix-vector multiplication.
- For efficiency, portability and convenience this scheme has been implemented using PETSc (http://www.mcs.anl.gov/petsc/).
- PETSc is a widely used, state-of-the-art open source numerical library for solution of (sparse) linear and nonlinear equations on distributed-memory computers (using MPI).
- The TMM driver code, interfaces to a variety of popular BGC models and TMs from various GCMs are freely available from: https://github.com/samarkhatiwala/tmm.
- The TMM code will run without modification on pretty much any computer from your laptop to a supercomputer.

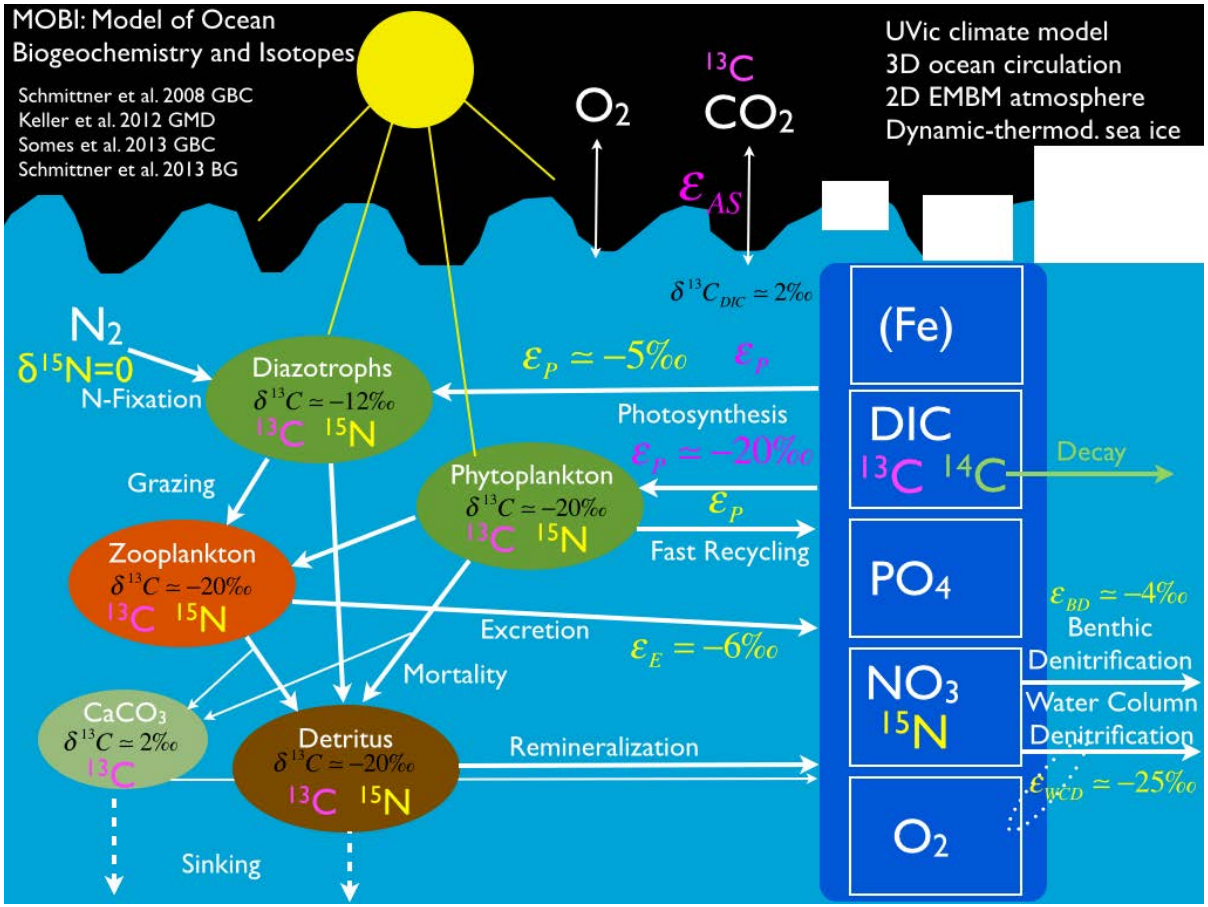
Using the TMM to constrain LGM circulation

- Use forcing from PMIP3 climate models to drive a common ocean model (UVic ESCM), extract TMs and then drive a common biogeochemical model

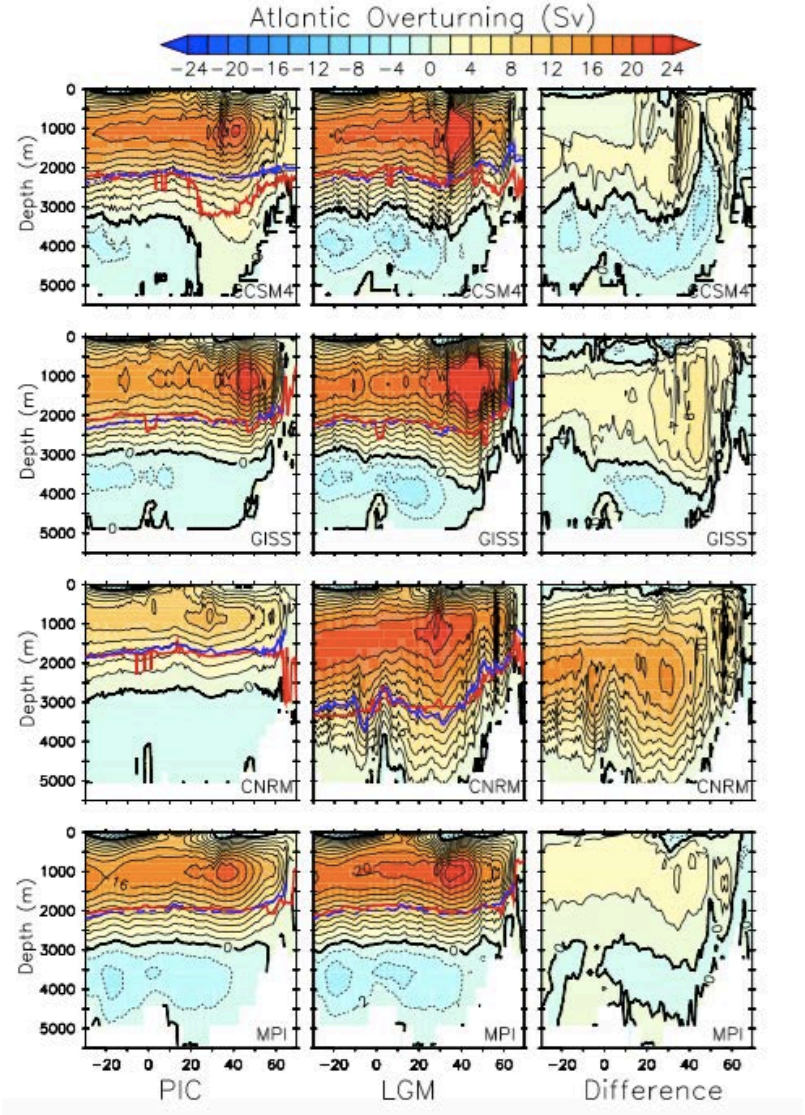


The Coupled Biogeochemical-Isotope Model

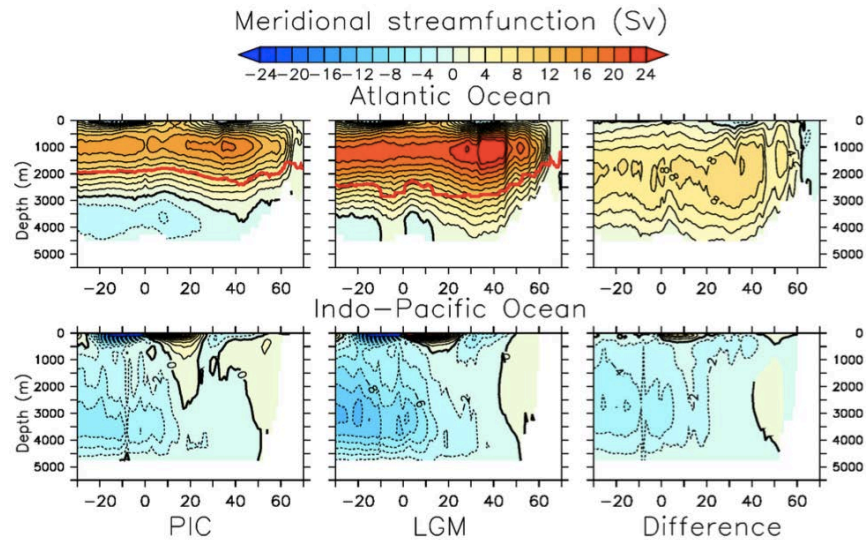
- **MOBI: Model of Ocean Biogeochemistry and Isotopes.**
- **MOBI incorporates ^{13}C and ^{15}N in all compartments of the carbon cycle; ^{14}C is included only in DIC.**
- **Pa/Th and Nd driven by biogeochemical fluxes from MOBI**



PMIP3 models systematically simulate a stronger and deeper AMOC in the LGM relative to that in their preindustrial (PI) control runs



PMIP3 ensemble mean overturning



PMIP3 ensemble mean AMOC stronger by ~41% in the LGM

Muglia and Schmittner, GRL 2015

This overall pattern is reproduced by the UVic ESCM when forced with wind stress from the PMIP3 models, with a ~39% increase in AMOC relative to a PI control run

Mean overturning in UVic ESCM forced by PMIP3 ensemble mean wind stress

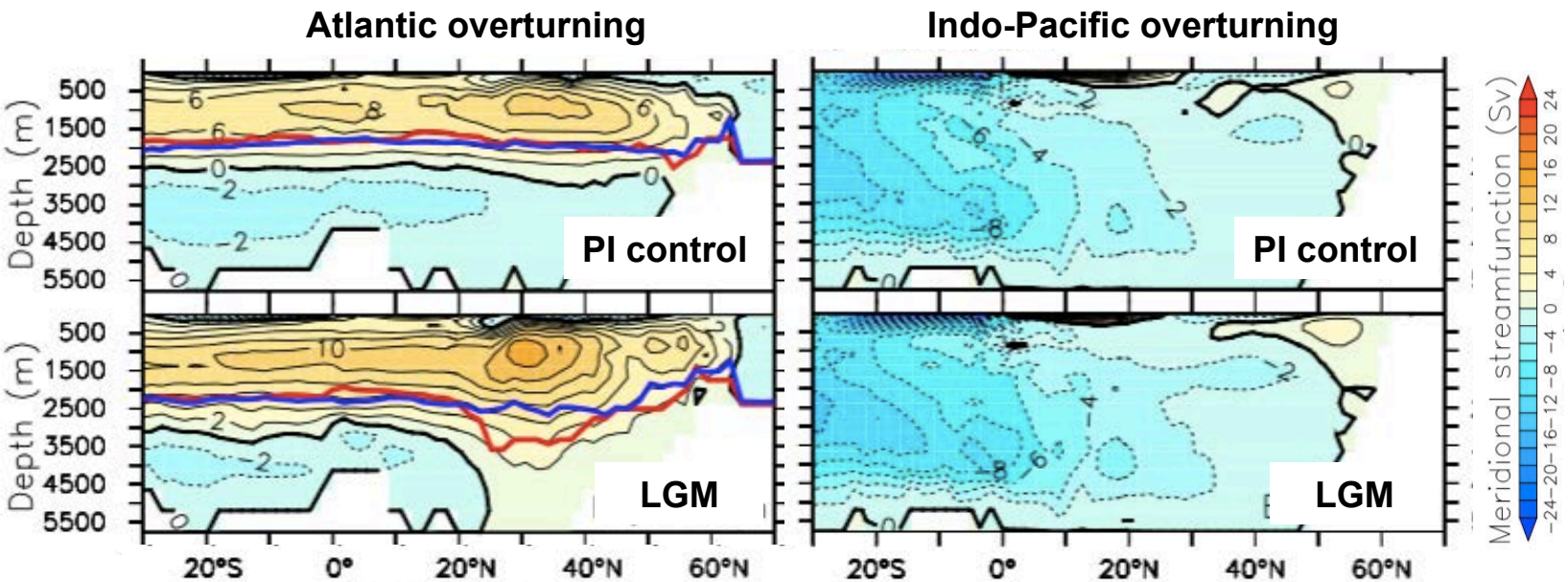


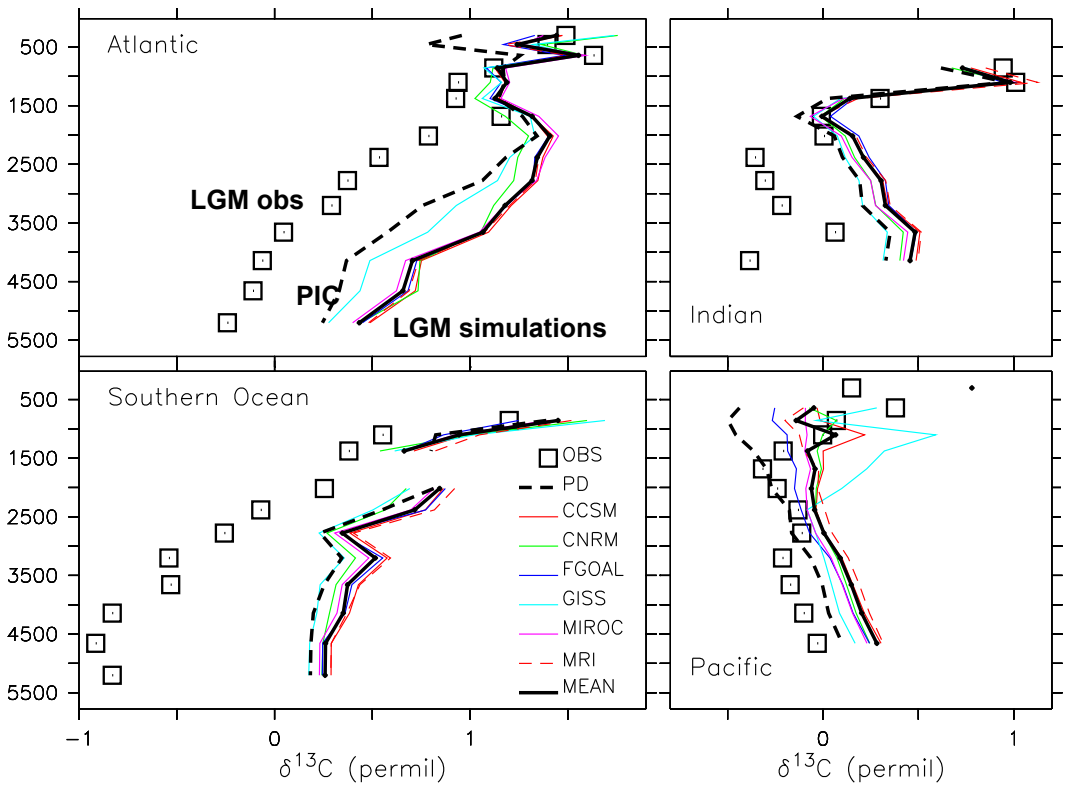
Table 2. Maximum Meridional Overturning, Percentage of Increment Between Wind Stress Experiments and Default Run, Salt Flux F_{salt} in the Atlantic Ocean, and Depth of the AMOC (All at 25°N) in the UVic Model Experiments[a]

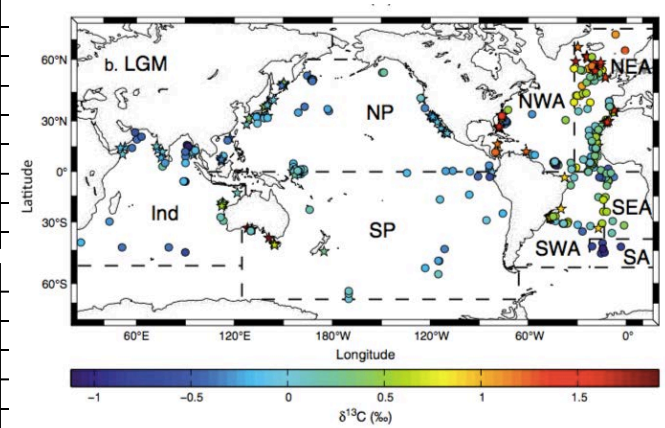
Model Case	AMOC (Sv)	Change (%)	F_{salt} (10^6 kg/s)	AMOC Depth (m)	Change (%)
Default	9.10	-	89.23	1905	-
CCSM4	13.56	49	99.32	3103	63
GISS	11.07	22	108.60	2203	16
CNRM	11.15	22	106.10	3300	73
MPI	12.13	33	102.70	3080	62
MIROC	13.33	46	98.78	3060	61
MRI	13.55	49	101.00	3068	61
FGOALS	13.84	52	97.77	3048	60
IPSL	12.78	40	96.60	3123	64

[a]Each row corresponds to wind stress anomalies from a different PMIP3 model. The top row corresponds to the default case. All numbers correspond to experiments using the PMIP3 ice sheet.

Muglia and Schmittner, 2015

$\delta^{13}C$ simulated by MOBI using circulations extracted from these PMIP3-forced runs appear inconsistent with LGM observations





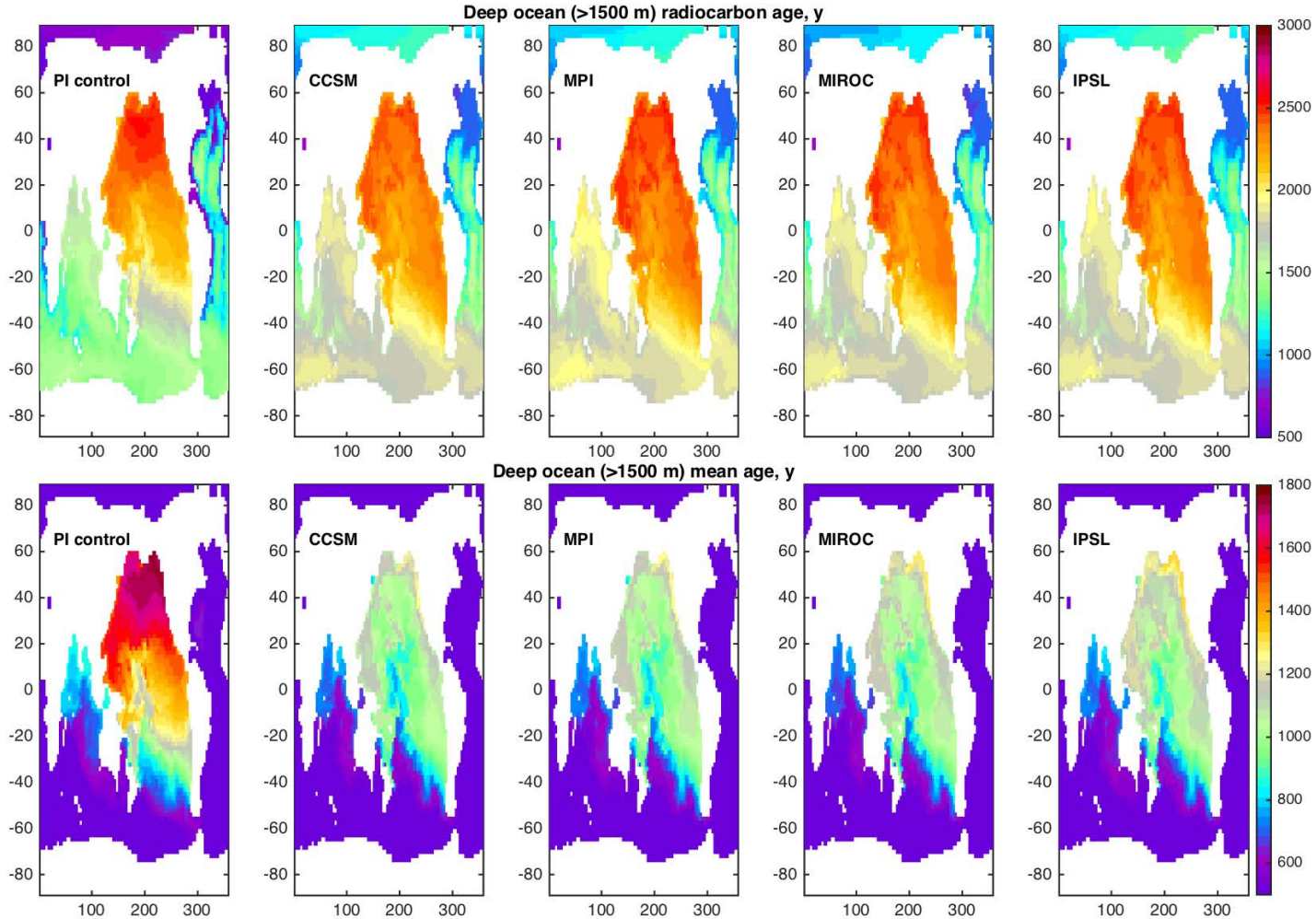
LGM data compiled by Peterson et al. 2014

Basin-averaged profiles of δ13C simulated using different PMIP3-based circulations

Simulated deep ocean radiocarbon ages are similar to or even slightly younger than present-day values, inconsistent with observations which suggest that deep waters were significantly depleted in ^{14}C during the LGM (e.g., Skinner and Shackleton, 2004; Robinson et al., 2005; Burke and Robinson, 2012; Sarnthein et al, 2013)

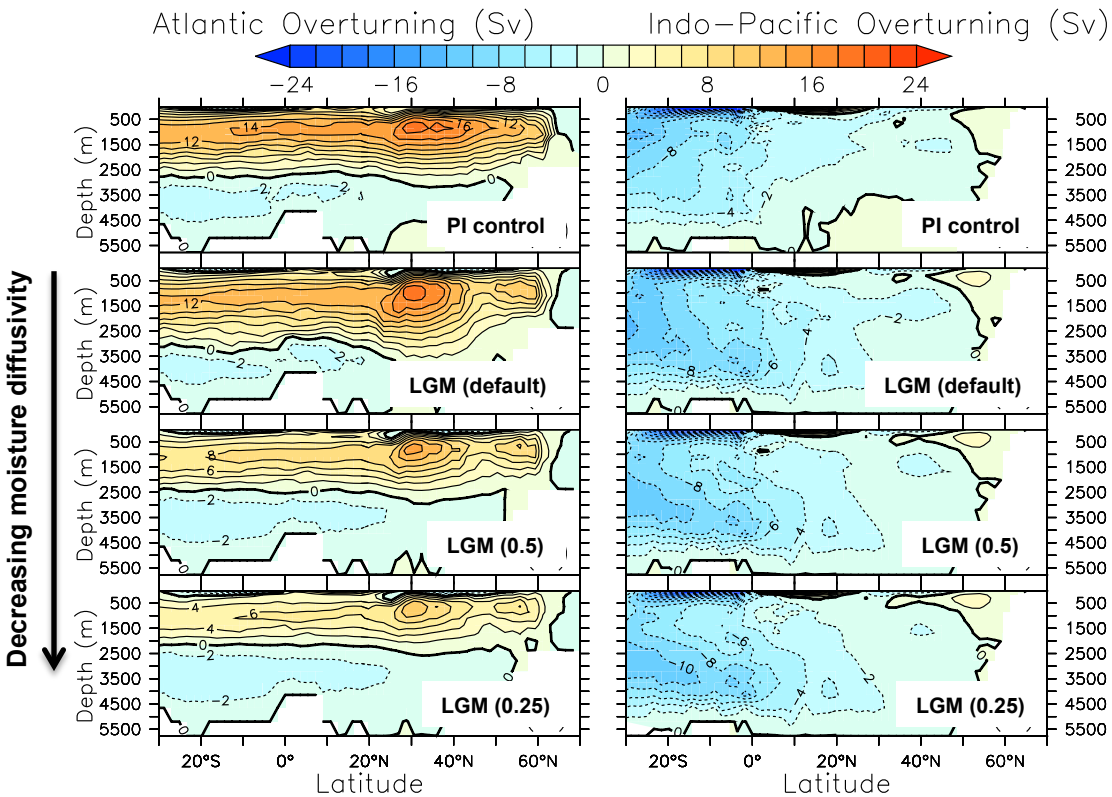
$\Delta^{14}C$ age

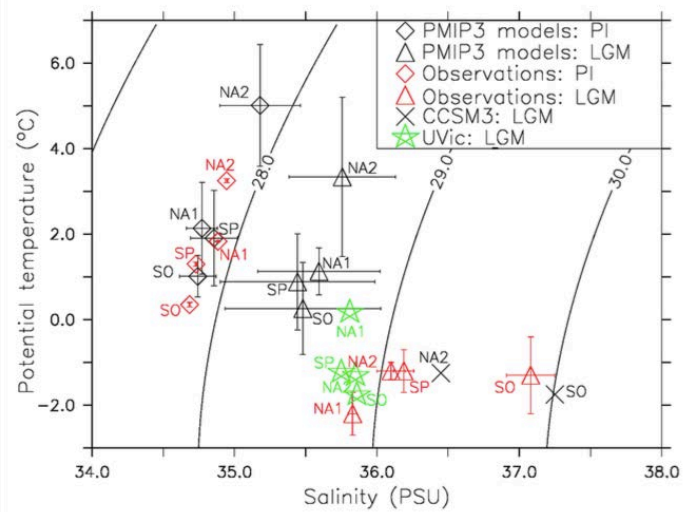
Ideal age



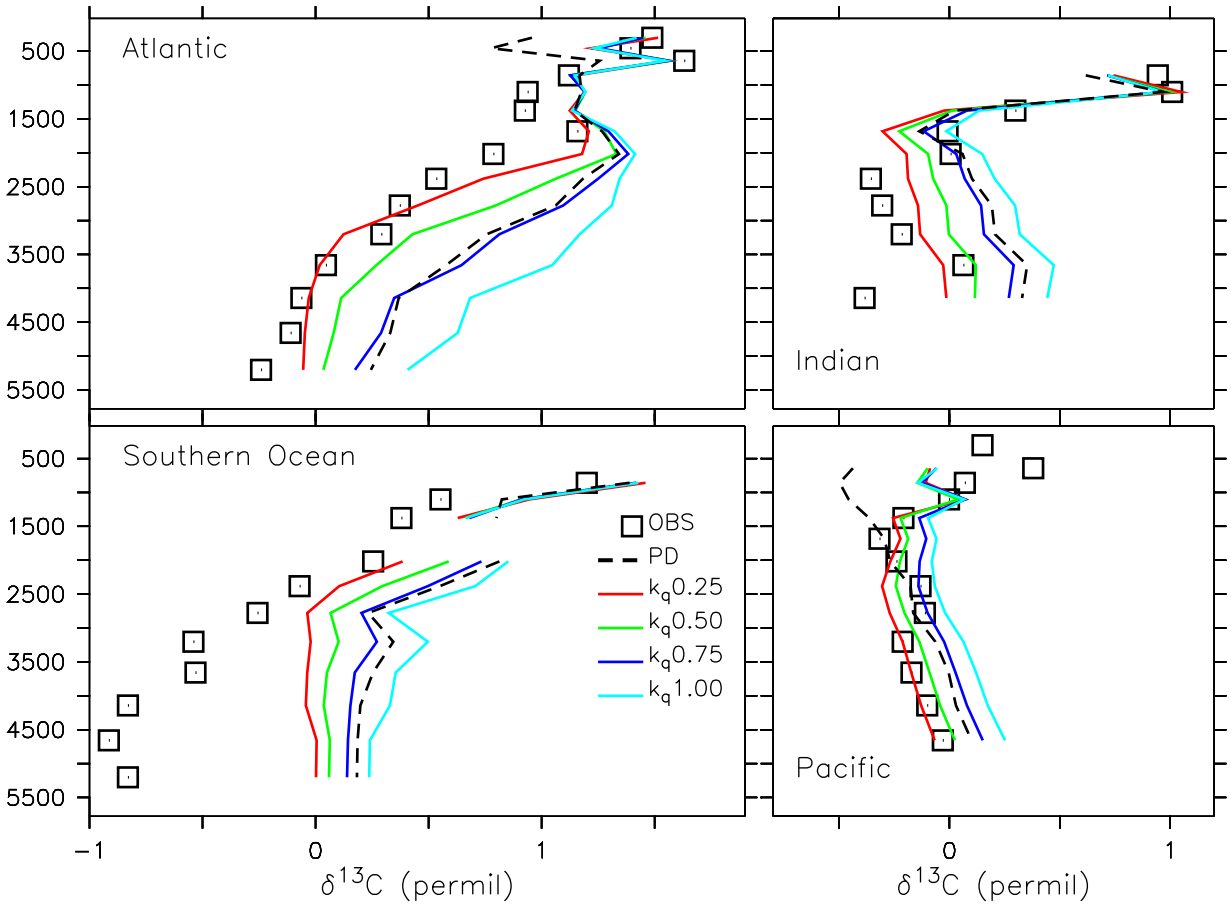
How to generate an equilibrium LGM state with weaker and shallower AMOC?

- **Deep circulation depends on poleward moisture transport (Saenko et al., 2003), which has been hypothesized to be lower during glacial periods (Sigman et al., 2007).**
- **A decrease in the SH eddy diffusivity for meridional moisture transport in UVic produces a weaker and shallower AMOC, more AABW in the Northern Hemisphere and saltier AABW than NADW.**

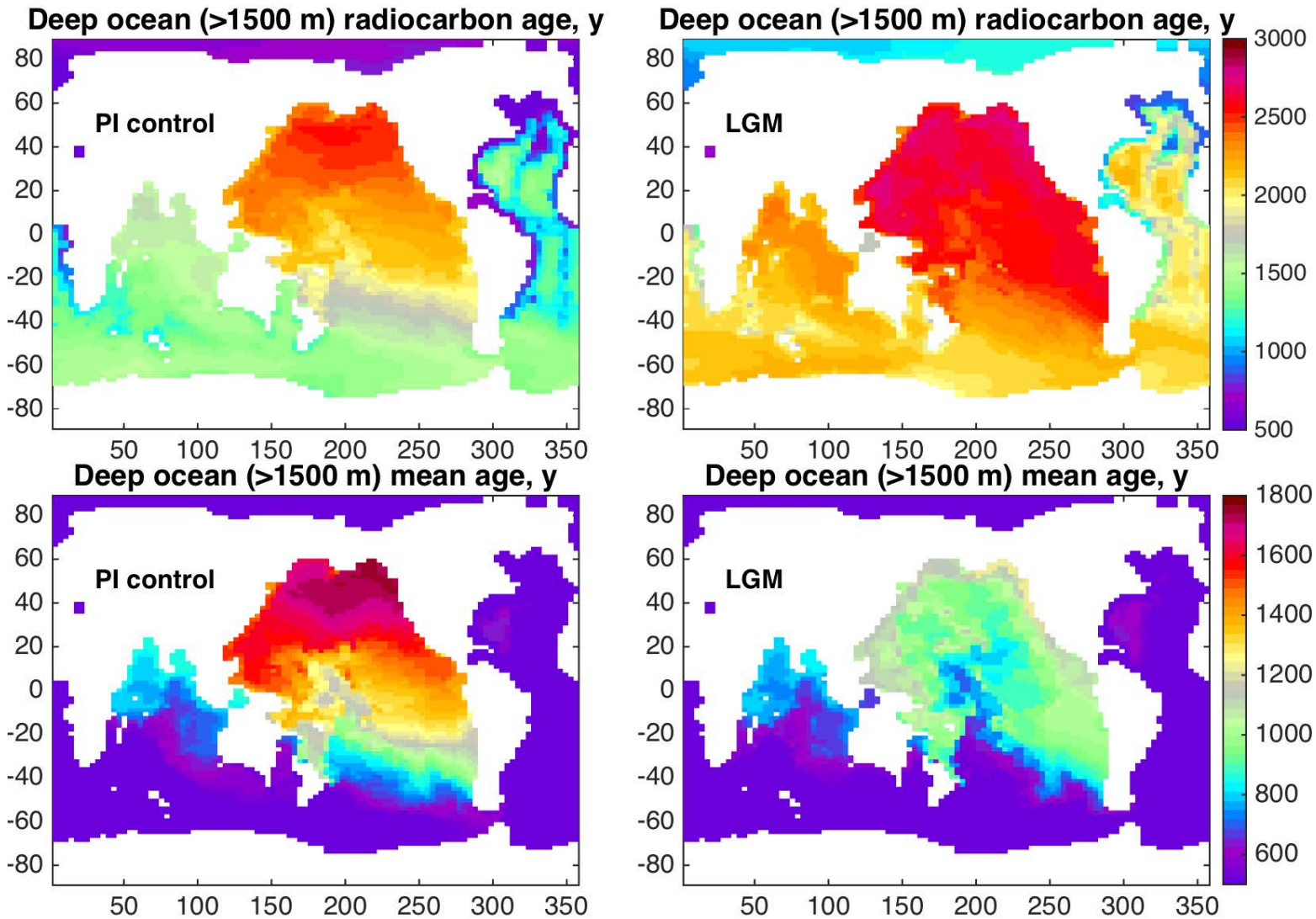




$\delta^{13}C$ simulated by MOBI using a circulation with reduced moisture diffusivity seems more consistent with LGM observations



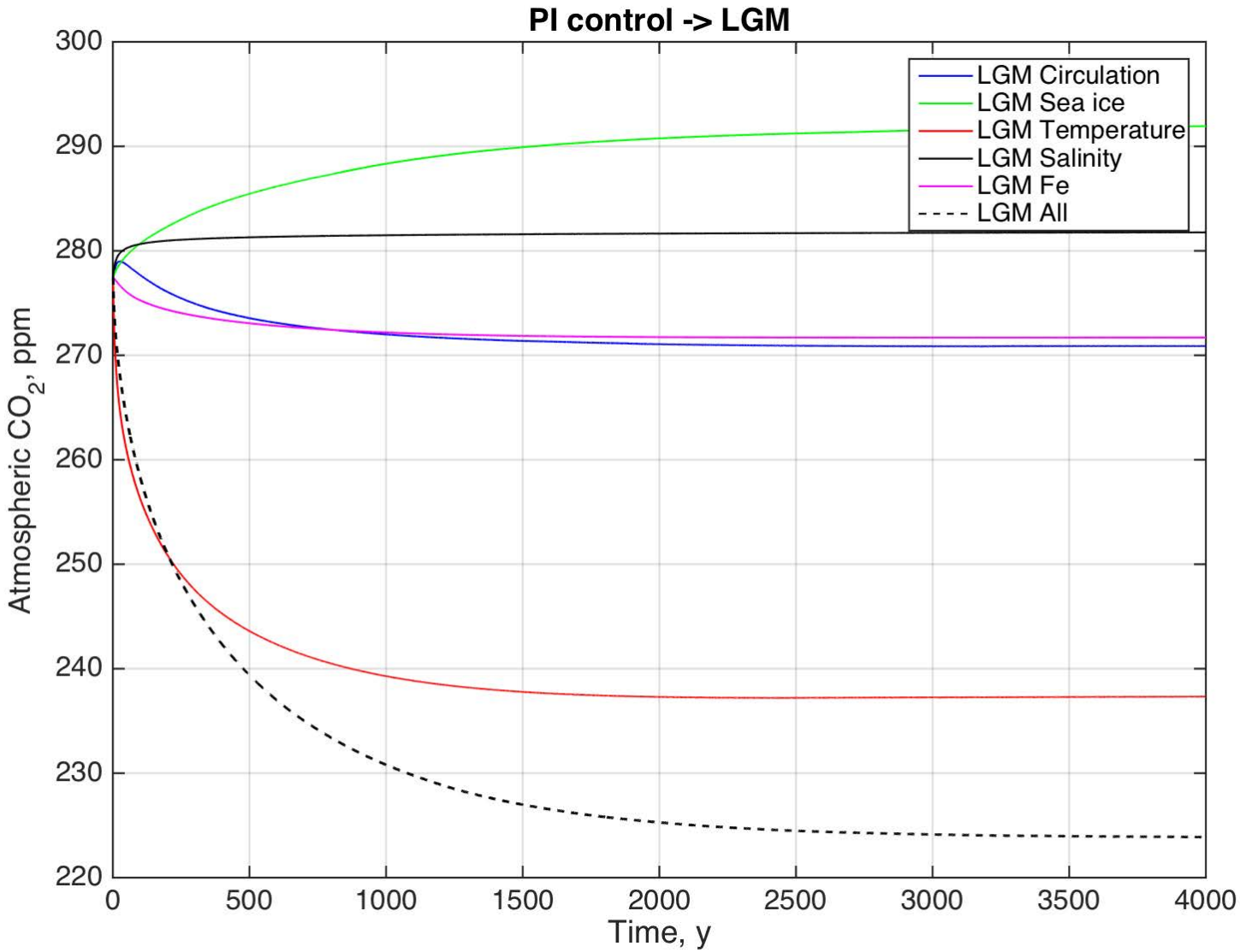
Simulated deep ocean radiocarbon ages are also now significantly older than the PI control run … although ventilation ages remain much younger



Can we say something about glacial-interglacial changes in atmospheric CO_2 from these simulations?

- Run MOBI to equilibrium with PI (LGM) circulation, etc. and fixed atmospheric CO_2 of 277 (189) ppm.
- Then replace various variables affecting biogeochemistry (circulation, temperature, sea ice, …) with their LGM (PI) values and allow the atmosphere and ocean to exchange CO_2.
- See how the partitioning of carbon changes between the ocean and atmosphere.

We change each parameter (circulation, sea ice, etc.) one at a time to see their individual effect



How does the biological pump respond to these perturbations?

We use the *P framework of Ito and Follows (2005) to separate changes in atmospheric CO_2 due to physical factors from those due to changes in the efficiency of the (soft tissue) biological pump**

$$P^* = \frac{\text{Mean regenerated phosphate concentration}}{\text{Mean phosphate concentration}}$$

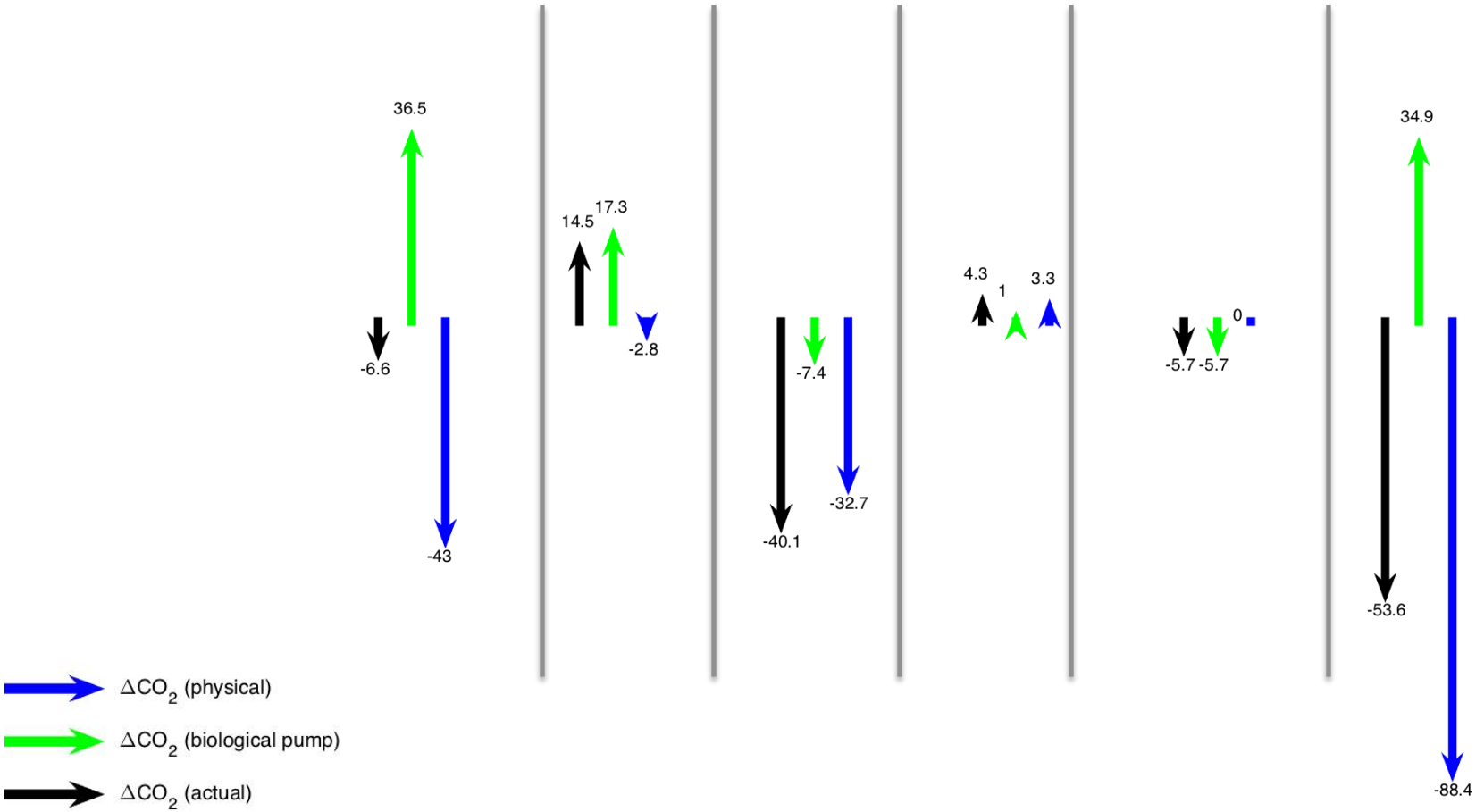
- **Larger values of *P** imply a more efficient biological pump and thus a lower atmospheric CO_2**
- **Ito and Follows use a simple theoretical argument to show that atmospheric CO_2 varies with P* as:**

$$\frac{\partial p\mathrm{CO}_2^{\mathrm{atm}}}{\partial P^*} = -\frac{V R_{\mathrm{C:P}} P_o}{M\gamma} \sim -312 \text{ ppm}$$

- **This sensitivity is model dependent; for MOBI it is ~ -623 ppm**

Effect of replacing various PI variables with their LGM values

	Circulation	Sea ice	Temp	Salt	Fe	All
ΔpCO_2	-6.6	14.5	-40.1	4.3	-5.7	-53.6
ΔP^*	-0.0584	-0.0277	0.0119	-0.0016	0.0092	-0.0559
$\Delta pCO_2/\Delta P^*$	112.2	-523.9	-3371.8	-2721.9	-623.8	958.3



Summary

- TMM is a fast, accurate, and easy to use framework for ocean biogeochemical modeling
- Orders of magnitude more efficient than GCMs or conventional "offline" models
- Direct computation of (periodic) steady state tracer distributions
- Easy to perform adjoint tracer and sensitivity calculations
- Convenient for rapid "prototyping" and testing of novel biogeochemical models
- Freely available from: https://github.com/samarkhatiwala/tmm