CAN RADIOCARBON RECORDS LEAD TO QUANTITATIVE ESTIMATES OF DEEP-OCEAN VENTILATION IN THE GEOLOGIC PAST?

A progress Report

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GOAL OF THIS RESEARCH

- The overarching goal of this research is to examine whether $\Delta^{14}C$ measurements on fossil benthic foraminifera & deep-sea corals (paleo-$\Delta^{14}C$ data) can provide quantitative information about deep ocean ventilation rates in the geologic past.

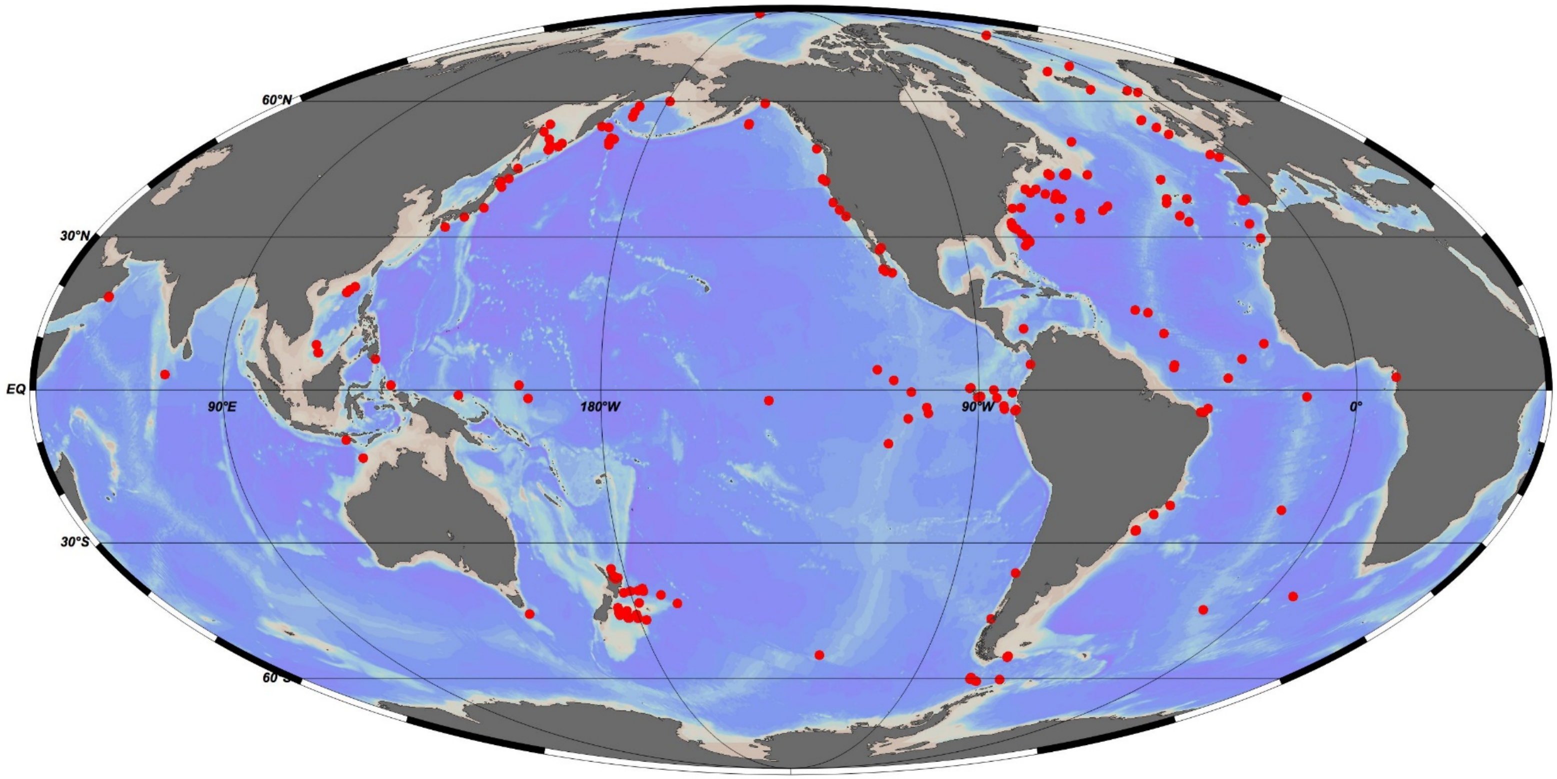
- In order to interpret paleo-$\Delta^{14}C$ data in terms of ventilation, a model (conceptual or mathematical) that relates $\Delta^{14}C$ to ventilation should be considered.

- Here we combine (i) paleo-$\Delta^{14}C$ data for the Atlantic Ocean and for the time span from 10 to 20 kyr BP with (ii) a $\Delta^{14}C$ transport model, using sequential methods of optimal estimation theory (a Kalman filter and a related smoother).

- The following specific question is addressed:

  Do Atlantic paleo-$\Delta^{14}C$ data require deglacial changes in deep ventilation?

COMPILATION OF PALEO-$\Delta^{14}C$ DATA



- *Number*: 1,698 paleo-$\Delta^{14}C$ data
- *Water depths*: 250 – 5000 m
- *Time span*: last 40,000 years

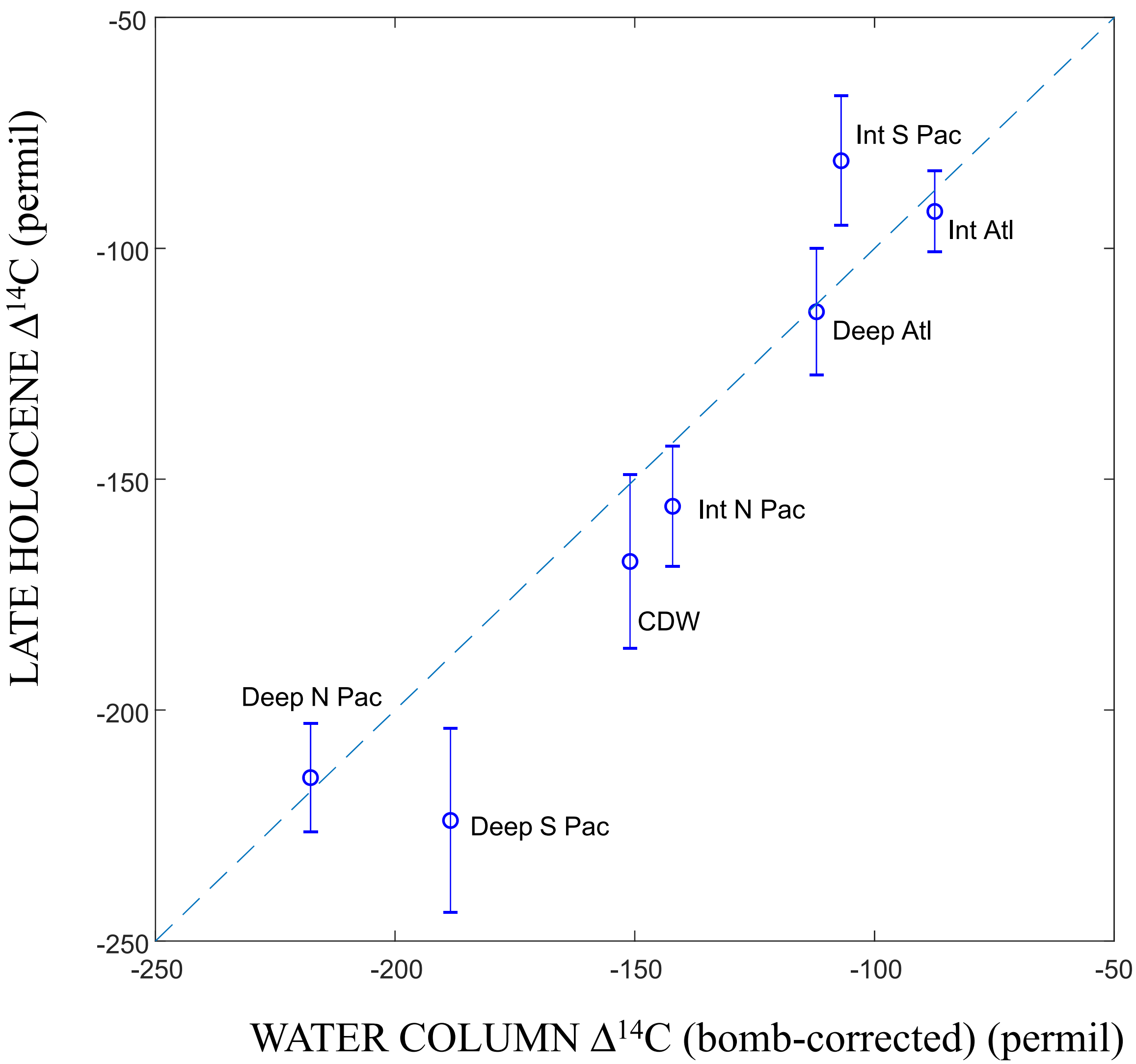
- Reliance on published chronologies
- Calibration to IntCal13 (Reimer *et al*. 2013)
- Data available at *https://www.ncdc.noaa.gov/paleo/study/21390*

COMPARISON BETWEEN FOSSIL & WATER COLUMN $\Delta^{14}C$ (next page)

- The next figure illustrates the relationship between $\Delta^{14}C$ measurements on fossil benthic foraminifera & deep-sea corals sampled from recent sediments (past 4 kyr) and water-column bomb-corrected $\Delta^{14}C$ measurements (Key et al. 2004).

- Circles show basin-averages and vertical bars show $\pm$ 1 standard errors. The dashed line is the line of perfect agreement.

COMPARISON BETWEEN FOSSIL & WATER COLUMN $\Delta^{14}C$ (BASIN AVERAGES)



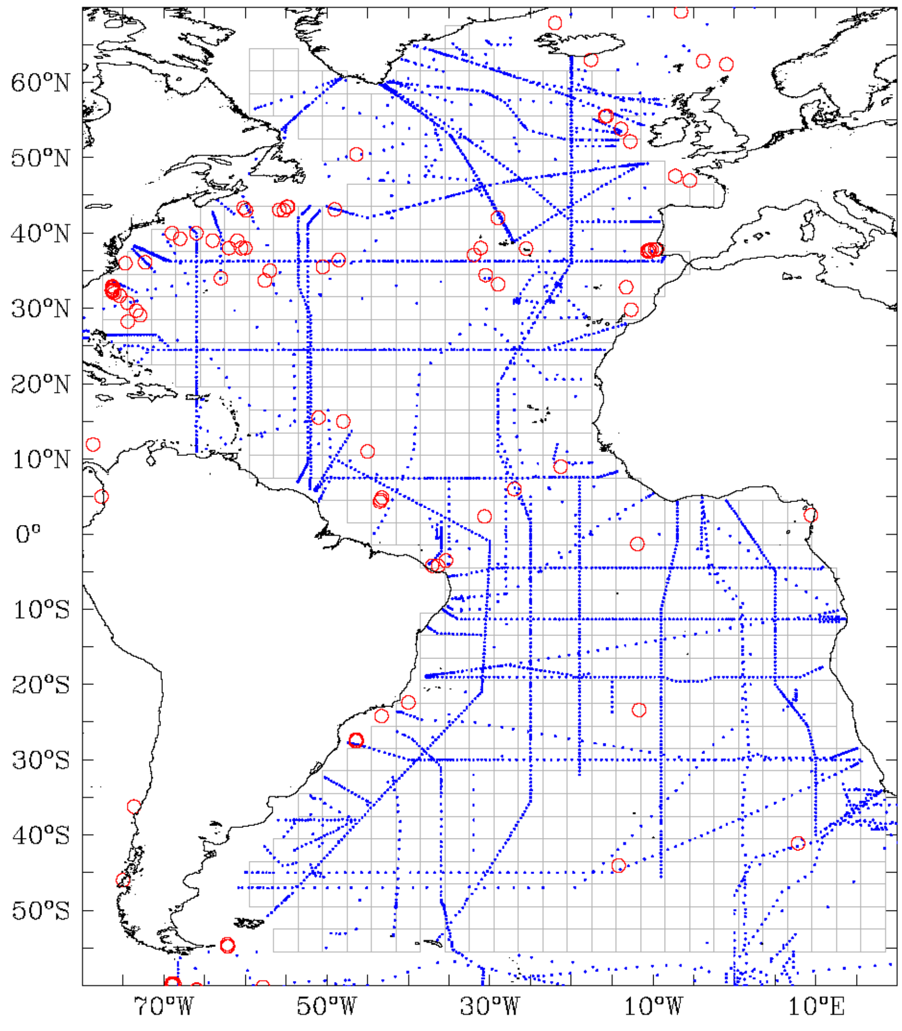
Zhao & Marchal (2019)

$\Delta^{14}C$ DATA DISTRIBUTIONS & MODEL GRID (next page)

- The next figure illustrates the regional domain considered for the present study. Shown are (i) the locations of water-column bomb-corrected $\Delta^{14}C$ data (Key et al. 2004), (ii) the locations of paleo-$\Delta^{14}C$ data (ongoing compilation), and (iii) the horizontal grid of the model.

- The vertical grid of the model (not shown) comprises four layers between 1000-2000 m, 2000-3000 m, 3000-4000 m, and 4000-5000 m. The layer between 0 – 1000 m includes boundary values of $\Delta^{14}C$.

$\Delta^{14}C$ DATA DISTRIBUTIONS & MODEL GRID



Water column bomb-corrected $\Delta^{14}C$ (Key et al. 2004)

Fossil $\Delta^{14}C$ (compilation of N. Zhao)

model grid

NEXT PAGES

In order to estimate the time-dependent ventilation state of the deep Atlantic during the deglaciation, both theoretical constraints and observational constraints are considered. For convenience, these constraints are written in vector-matrix form (state-space notation).

THEORETICAL CONSTRAINTS

1) Transport model for $C \equiv \Delta^{14}\mathrm{C}$:

$$\boxed{\frac{\partial C}{\partial t} + \nabla \cdot (\boldsymbol{u}C) = -\lambda C + \epsilon_C}$$

where $\boldsymbol{u} = (u, v, w)$ is the velocity vector
λ is the ^{14}C radioactive decay constant
ϵ_c is the equation error

2) Probability model for – boundary C values
– velocity $\boldsymbol{u}$

$$\boxed{\begin{aligned} \mathrm{d}C_B &= \epsilon_B \mathrm{d}t \\ \mathrm{d}\boldsymbol{u} &= \boldsymbol{\epsilon_u} \mathrm{d}t \end{aligned}}$$

where $(\epsilon_B, \boldsymbol{\epsilon_u})$ are equation errors

THEORETICAL CONSTRAINTS

1) Transport model for $C \equiv \Delta^{14}\mathrm{C}$:

$$\frac{\partial C}{\partial t} + \nabla \cdot (\boldsymbol{u}C) = -\lambda C + \epsilon_C$$

where $\boldsymbol{u} = (u, v, w)$ is the velocity vector
λ is the ^{14}C radioactive decay constant
ϵ_c is the equation error

state vector

$$\boldsymbol{x}_i = \boldsymbol{f}(\boldsymbol{x}_{i-1}) + \boldsymbol{e}_i^{(k)}$$

function vector

error vector

2) Probability model for – boundary C values
– velocity $\boldsymbol{u}$

$$\mathrm{d}C_B = \epsilon_B \mathrm{d}t$$
$$\mathrm{d}\boldsymbol{u} = \boldsymbol{\epsilon_u} \mathrm{d}t$$

where $(\epsilon_B, \boldsymbol{\epsilon_u})$ are equation errors

OBSERVATIONAL CONSTRAINTS

state vector

observation vector
(paleo-Δ^{14}C data)

$$\boldsymbol{z}_i = \boldsymbol{H}_i \boldsymbol{x}_i + \boldsymbol{e}_i^{(o)}$$

error vector

observation matrix

ASSUMPTIONS ABOUT EQUATION ERRORS

- Transition equation

$$\boxed{\boldsymbol{x}_i = \boldsymbol{f}(\boldsymbol{x}_{i-1}) + \boldsymbol{e}_i^{(k)}}$$

- Observation equation

$$\boxed{\boldsymbol{z}_i = \boldsymbol{H}_i \boldsymbol{x}_i + \boldsymbol{e}_i^{(o)}}$$

- Assumptions about equation errors (E = expected value)

$$E\left[\boldsymbol{e}_i^{(k)}\right] = \boldsymbol{0} \qquad E\left[\boldsymbol{e}_i^{(k)} \boldsymbol{e}_j^{(k)}\right] = \boldsymbol{Q}_i \delta_{ij}$$

$$E\left[\boldsymbol{e}_i^{(o)}\right] = \boldsymbol{0} \qquad E\left[\boldsymbol{e}_i^{(o)} \boldsymbol{e}_j^{(o)}\right] = \boldsymbol{R}_i \delta_{ij}$$

where $\delta_{ij} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}$

where $\boldsymbol{Q}_i$ & $\boldsymbol{R}_i$ are covariance matrices for equation errors & data errors

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The theoretical and observational constraints are combined using two sequential methods used for state estimation: a linearized Kalman filter and a linearized smoother.

A FEW DEFINITIONS

$\hat{\boldsymbol{x}}_i(-)$: state estimate at time i constrained by data at times $0 < i$

$\hat{\boldsymbol{x}}_i(+)$: state estimate at time i constrained by data at times $0 \leq i$ (filtering solution)

$\hat{\boldsymbol{x}}_i$: state estimate at time i constrained by data at times $0 \leq i \leq N$ (smoothing solution)

$\boldsymbol{P}_i(-)$: error covariance matrix for $\hat{\boldsymbol{x}}_i(-)$

$\boldsymbol{P}_i(+)$: error covariance matrix for $\hat{\boldsymbol{x}}_i(+)$

$\boldsymbol{P}_i$ error covariance matrix for $\hat{\boldsymbol{x}}_i$

LINEARIZED KALMAN FILTER

- Extrapolation (forecast)

$$\hat{\boldsymbol{x}}_i(-) = \boldsymbol{f}[\hat{\boldsymbol{x}}_{i-1}(+)]$$

$$\boxed{\boldsymbol{P}_i(-) = \left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)_{\hat{\boldsymbol{x}}_0(+)} \boldsymbol{P}_{i-1}(+) \left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)^T_{\hat{\boldsymbol{x}}_0(+)} + \boldsymbol{Q}_{i-1}}$$

computationally expensive

- Update (analysis)

$$\hat{\boldsymbol{x}}_i(+) = \hat{\boldsymbol{x}}_i(-) + \boldsymbol{K}_i[\boldsymbol{z}_i - \boldsymbol{H}_i\hat{\boldsymbol{x}}_i(-)]$$

$$\boldsymbol{P}_i(+) = [\boldsymbol{I} - \boldsymbol{K}_i\boldsymbol{H}_i]\boldsymbol{P}_i(-)$$

where

$$\boldsymbol{K}_i = \boldsymbol{P}_i(-)\boldsymbol{H}_i^T \left[\boldsymbol{H}_i\boldsymbol{P}_i(-)\boldsymbol{H}_i^T + \boldsymbol{R}_i\right]^{-1}$$ is the Kalman gain

Bryson & Ho (1975)

LINEARIZED SMOOTHER

$$\hat{\boldsymbol{x}}_i = \hat{\boldsymbol{x}}_i(+) - \boldsymbol{C}_i[\hat{\boldsymbol{x}}_{i+1}(-) - \hat{\boldsymbol{x}}_{i+1}]$$

$$\boxed{\boldsymbol{P}_i = \boldsymbol{P}_i(+) - \boldsymbol{C}_i[\boldsymbol{P}_{i+1}(-) - \boldsymbol{P}_{i+1}]\boldsymbol{C}_i^T}$$

computationally expensive

where

$$\boxed{\boldsymbol{C}_i = \boldsymbol{P}_i(+)\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)^T_{\hat{x}_0(+)} [\boldsymbol{P}_{i+1}(-)]^{-1}}$$

computationally expensive

Bryson & Ho (1975)

NEXT PAGES

To reduce the computational cost of ocean state estimation, we use an approximate filter (*Fukumori & Malanotte-Rizzoli* 1995) and an approximate smoother (*Fukumori* 1995). Both methods rely on the *reduced-state approximation* to compute state error covariances.

REDUCED-STATE APPROXIMATION

- Reduced state, $\boldsymbol{x}_i'$

$$\boldsymbol{x}_i \approx \boldsymbol{B}\boldsymbol{x}_i' \quad \longleftrightarrow \quad \boldsymbol{x}_i' \approx \boldsymbol{B}^{\#}\boldsymbol{x}_i$$

where $\boldsymbol{x}_i \in \mathbb{R}^N$

$\boldsymbol{x}_i' \in \mathbb{R}^{N'}$ where $N' \ll N$

$\boldsymbol{B} \in \mathbb{R}^{N\times N'}$ is a transformation matrix (mapping)

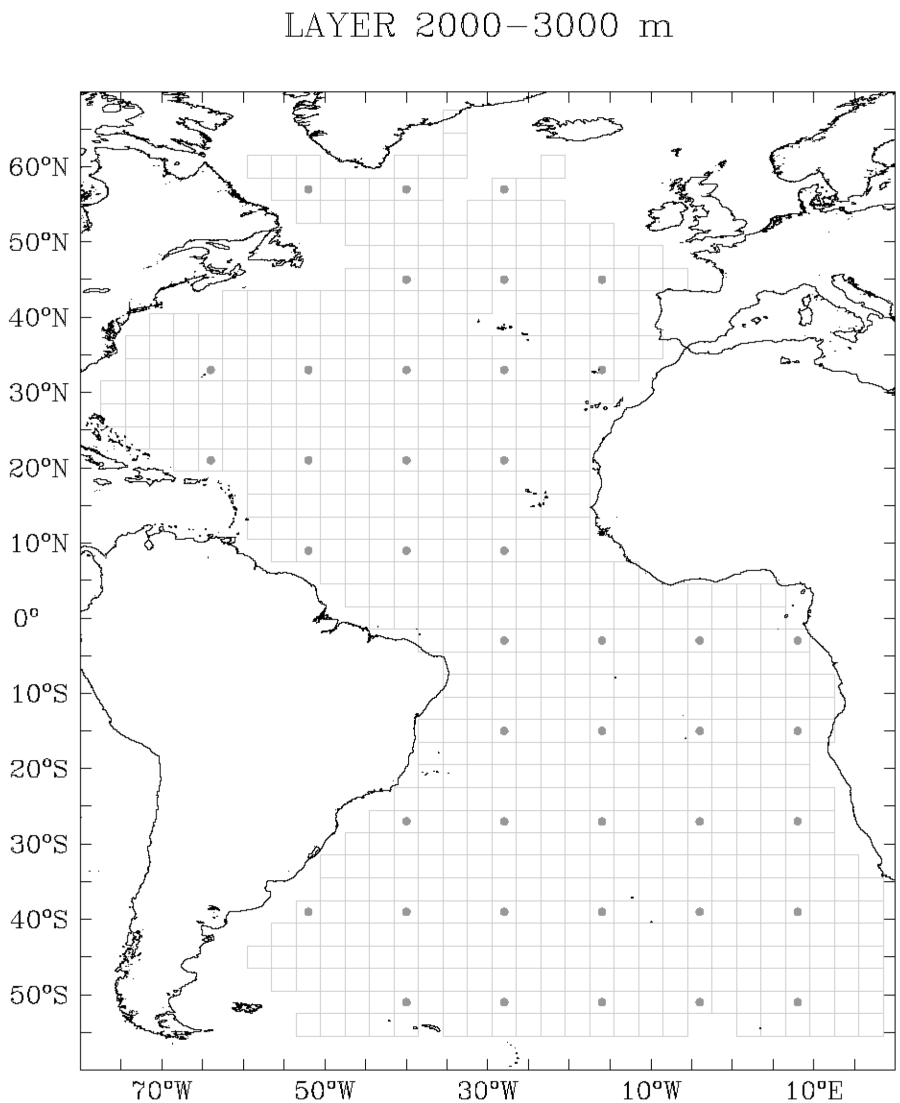
$\boldsymbol{B}^{\#} \in \mathbb{R}^{N'\times N}$ is the pseudo-inverse of $\boldsymbol{B}$

- Error covariance matrix for reduced state, $\boldsymbol{P}_i'$

$$\boldsymbol{P}_i \approx \boldsymbol{B}\boldsymbol{P}_i'\boldsymbol{B}^T \quad \longleftrightarrow \quad \boldsymbol{P}_i' \approx \boldsymbol{B}^{\#}\boldsymbol{P}_i\boldsymbol{B}^{\#T}$$

Fukumori & Malanotte-Rizzoli (1995)

REDUCED-STATE APPROXIMATION



In our study, the “reduced state” includes oceanic variables defined on a horizontal grid that is coarser than that for the full state. This map shows the grid for the full state and the $\Delta^{14}C$-carrying points for the reduced state, for the layer 2000-3000 m.

□ Grid for full state $(\boldsymbol{x}_i)$

● $\Delta^{14}C$ pts for reduced state $(\boldsymbol{x}'_i)$

NEXT PAGES

The reduced-state approximation is used to derive approximate versions of the filter and smoother equations that can be solved with relatively small computational resources.

APPROXIMATE LINEARIZED KALMAN FILTER

- Extrapolation (forecast)

$$\hat{\boldsymbol{x}}_i(-) = \boldsymbol{f}[\hat{\boldsymbol{x}}_{i-1}(+)]$$

$$\boxed{\boldsymbol{P}'_i(-) = \boldsymbol{B}^{\#}\left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)_{\hat{\boldsymbol{x}}_0(+)} \boldsymbol{B}\boldsymbol{P}'_{\boldsymbol{i-1}}(+)\boldsymbol{B}^T \left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)^T_{\hat{\boldsymbol{x}}_0(+)} \boldsymbol{B}^{\#T} + \boldsymbol{B}^{\#}\,\boldsymbol{Q}_{i-1}\,\boldsymbol{B}^{\#T}}$$

computationally cheap

- Update (analysis)

$$\hat{\boldsymbol{x}}_i(+) = \hat{\boldsymbol{x}}_i(-) + \boldsymbol{K}_i[\boldsymbol{z}_i - \boldsymbol{H}_i\hat{\boldsymbol{x}}_i(-)]$$

$$\boldsymbol{P}'_i(+) = [\boldsymbol{I} - \boldsymbol{B}^{\#}\boldsymbol{K}_i\boldsymbol{H}_i\boldsymbol{B}]\boldsymbol{P}'_i(-)$$

where

$$\boldsymbol{K}_i = \boldsymbol{B}\boldsymbol{P}'_i(-)\boldsymbol{B}^T\boldsymbol{H}_i^T\left[\boldsymbol{H}_i\boldsymbol{B}\boldsymbol{P}'_i(-)\boldsymbol{B}^T\boldsymbol{H}_i^T + \boldsymbol{R}_i\right]^{-1}$$

APPROXIMATE LINEARIZED SMOOTHER

$$\hat{\boldsymbol{x}}_i = \hat{\boldsymbol{x}}_i(+) - \boldsymbol{C}_i[\hat{\boldsymbol{x}}_{i+1}(-) - \hat{\boldsymbol{x}}_{i+1}]$$

$$\boxed{\boldsymbol{P}'_i = \boldsymbol{P}'_i(+) - \boldsymbol{C}'_i[\boldsymbol{P}'_{i+1}(-) - \boldsymbol{P}'_{i+1}]\boldsymbol{C}'^T_i}$$

computationally cheap

where

$$\boldsymbol{C}_i = \boldsymbol{B}\boldsymbol{P}'_i(+)\boldsymbol{B}^T \left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)^T_{\hat{x}_0(+)} \boldsymbol{B}^{\#T}[\boldsymbol{P}'_{i+1}(-)]^{-1}\boldsymbol{B}^{\#}$$

$$\boldsymbol{C}'_i = \boldsymbol{P}'_i(+)\boldsymbol{B}^T \left(\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{x}}\right)^T_{\hat{x}_0(+)} \boldsymbol{B}^{\#T}[\boldsymbol{P}'_{i+1}(-)]^{-1}$$

computationally cheap

using

$$[\boldsymbol{P}_i]^{-1} = \boldsymbol{B}^{*T}[\boldsymbol{P}'_i]^{-1}\boldsymbol{B}^*$$

NEXT PAGES

The approximate linearized filter and smoother are applied to test the following hypothesis:

H1: paleo-$\Delta^{14}C$ records are consistent with modern circulation in the deep Atlantic

ESTIMATION OF MODERN CIRCULATION

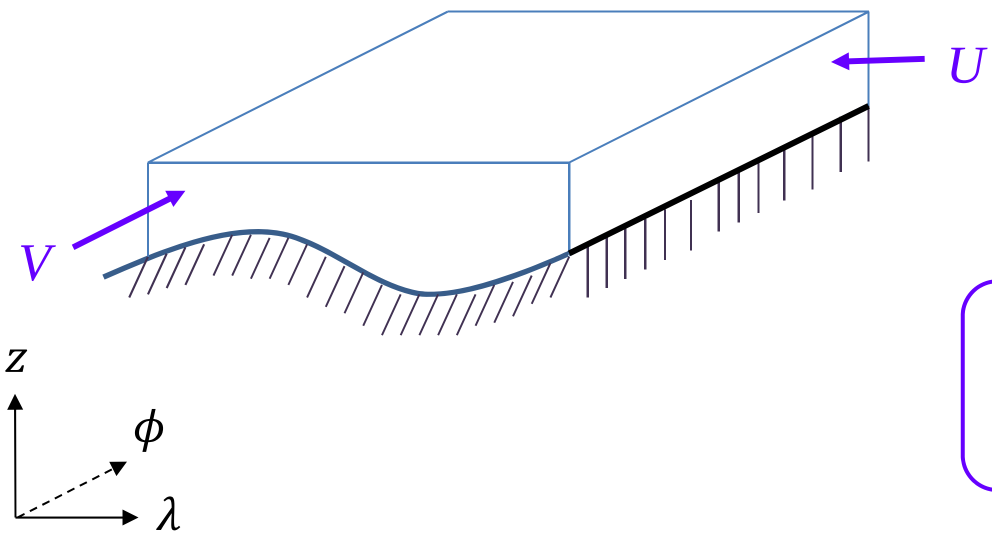
An estimate of modern circulation in the deep Atlantic is obtained from observational & dynamical constraints using weighted least-squares (e.g., Wunsch 2006):

- Observational constraints:
  - Water ρ climatology (WOA 2013)
  - Volume transports of NADW, AABW, MOW at specific locations
  - Zonally integrated transport at 32°S, 24°N, 36°N
- Dynamical constraints:
  - Thermal wind relationships
  - Linear vorticity balance
  - Mass balance equation

NEXT PAGE

The next page describes the calculation of the ventilation time scale (τ) and of its error estimate (σ_τ) in different layers, which are obtained from our estimate of modern circulation.

VENTILATION TIME SCALE, τ



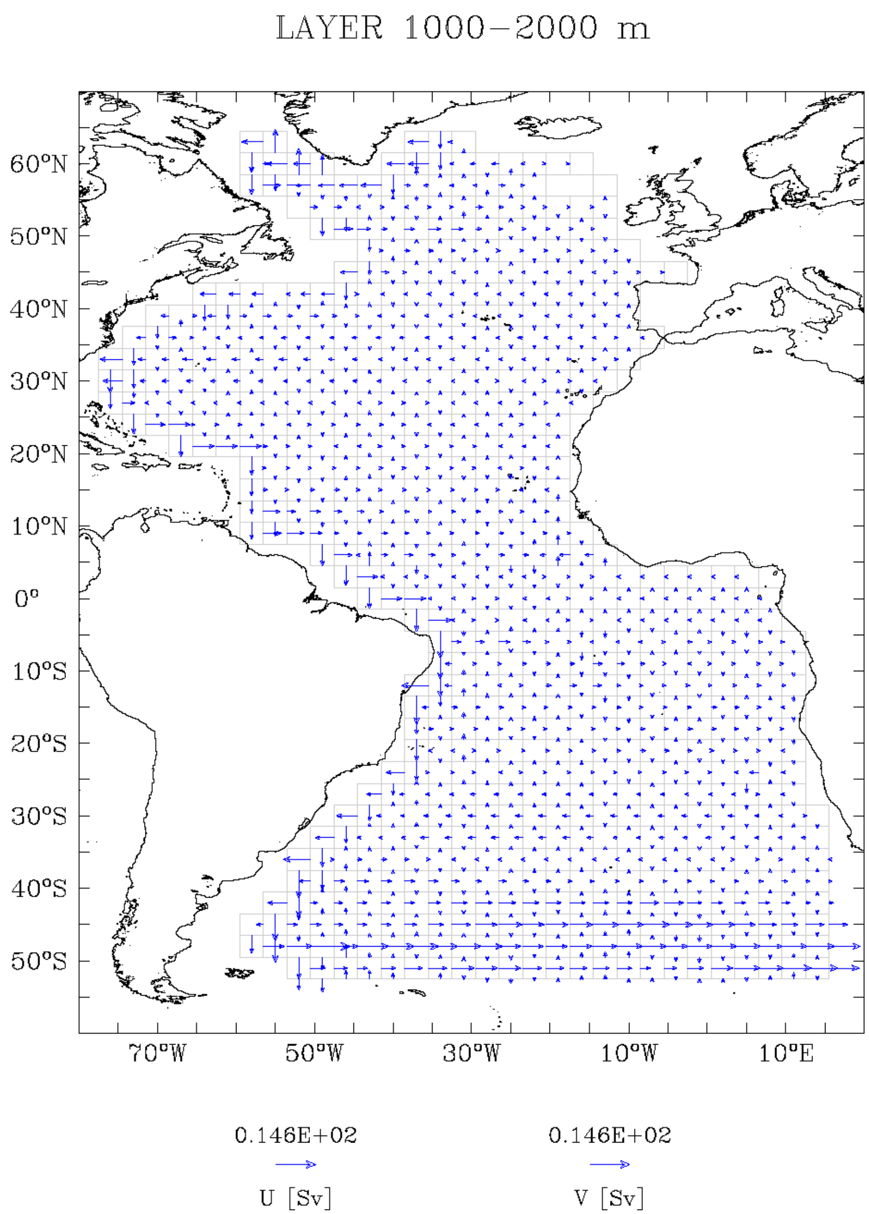
$$\tau = \frac{Volume}{\sum_i |U_i| + \sum_i |V_i|}$$

$$\sigma_\tau = \tau \frac{\sigma_\Sigma}{\Sigma}$$

where

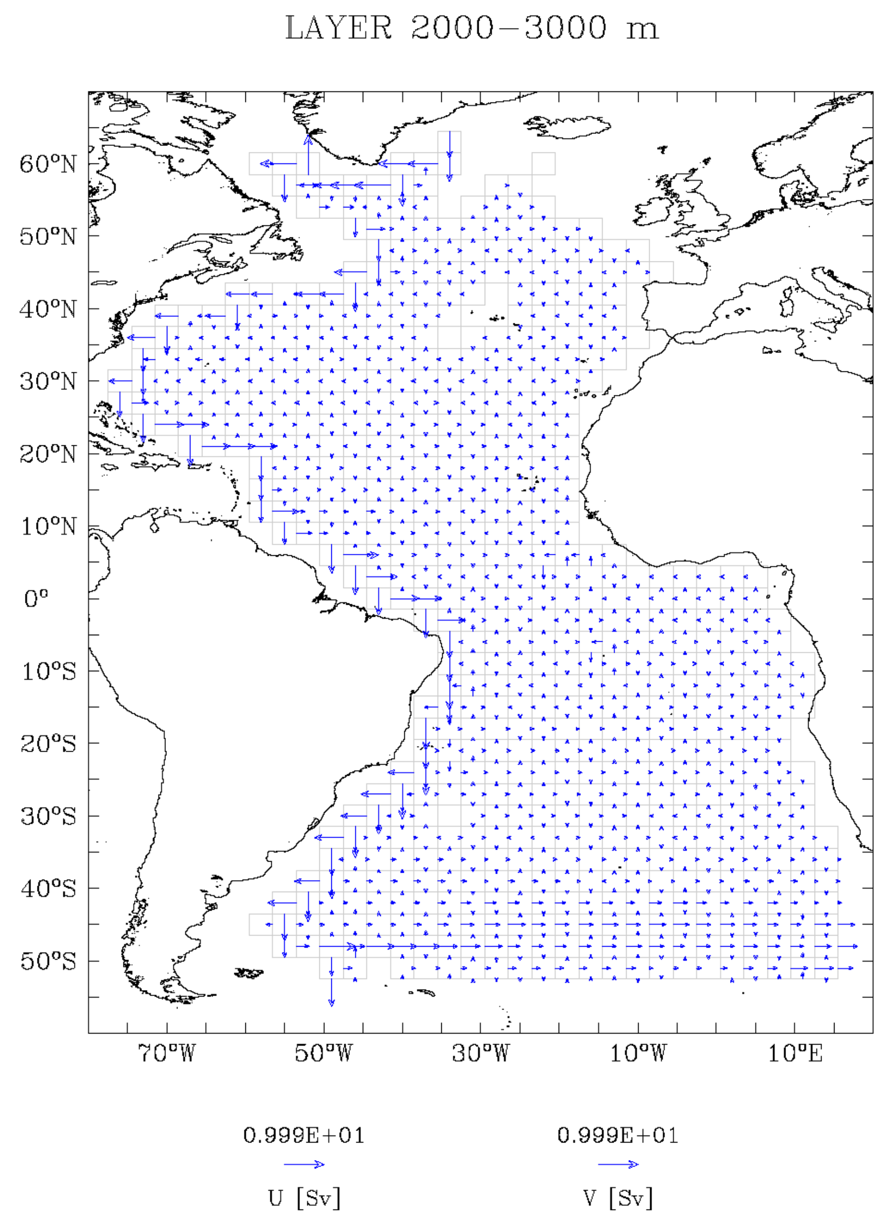
$$\left\{ \begin{array}{l} \Sigma \equiv \sum_i |U_i| + \sum_i |V_i| \equiv \sum_i |\mathcal{V}_i| \\ \sigma_\Sigma = \sum_i \left(\frac{\partial \Sigma}{\partial \mathcal{V}_i} \sigma_{\mathcal{V}_i} \right)^2 + 2 \sum_i \sum_j \frac{\partial \Sigma}{\partial \mathcal{V}_i} \frac{\partial \Sigma}{\partial \mathcal{V}_j} \sigma^2_{\mathcal{V}_i \mathcal{V}_j} \end{array} \right.$$

ESTIMATED TRANSPORTS & VENTILATION IN MODERN DEEP ATLANTIC



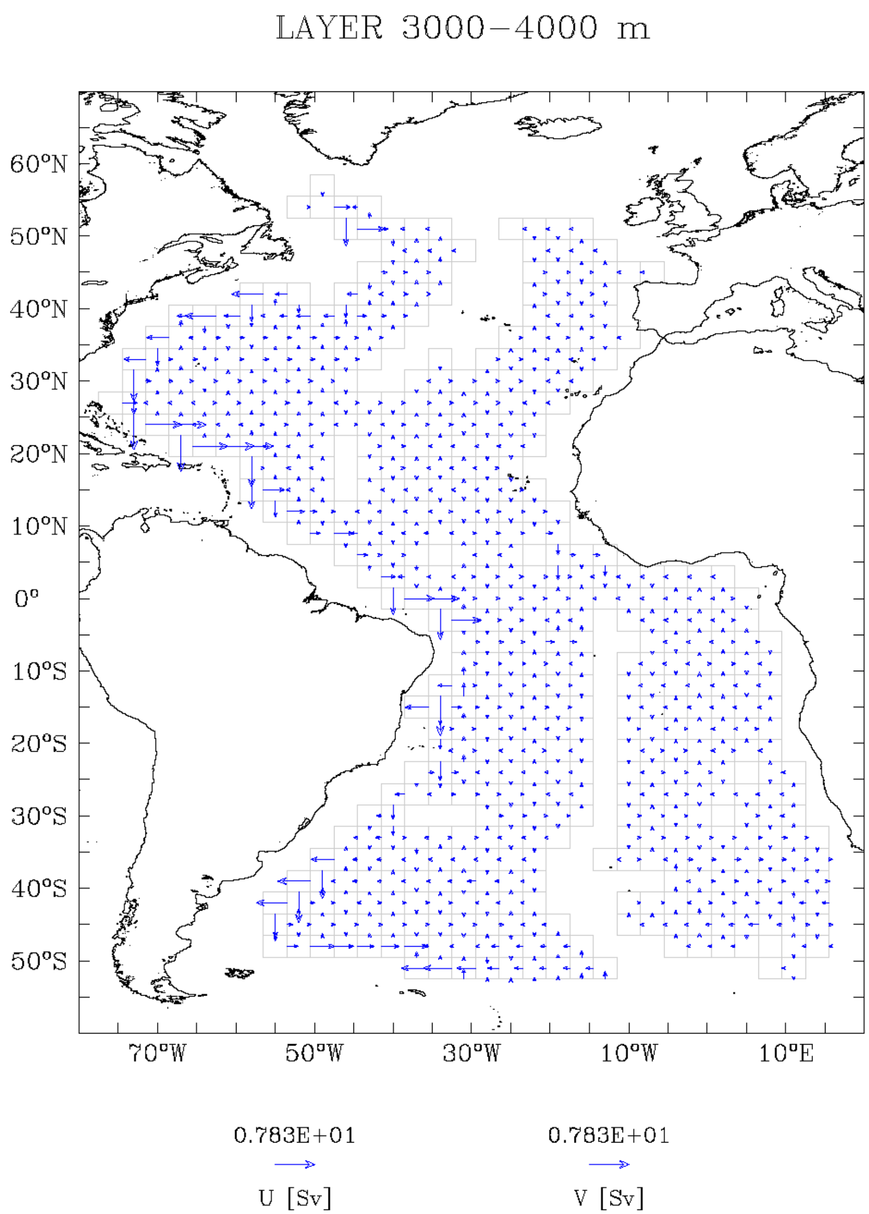
$$\tau \pm \sigma_{\tau} = 29 \pm 2 \text{ yr}$$

ESTIMATED TRANSPORTS & VENTILATION IN MODERN DEEP ATLANTIC



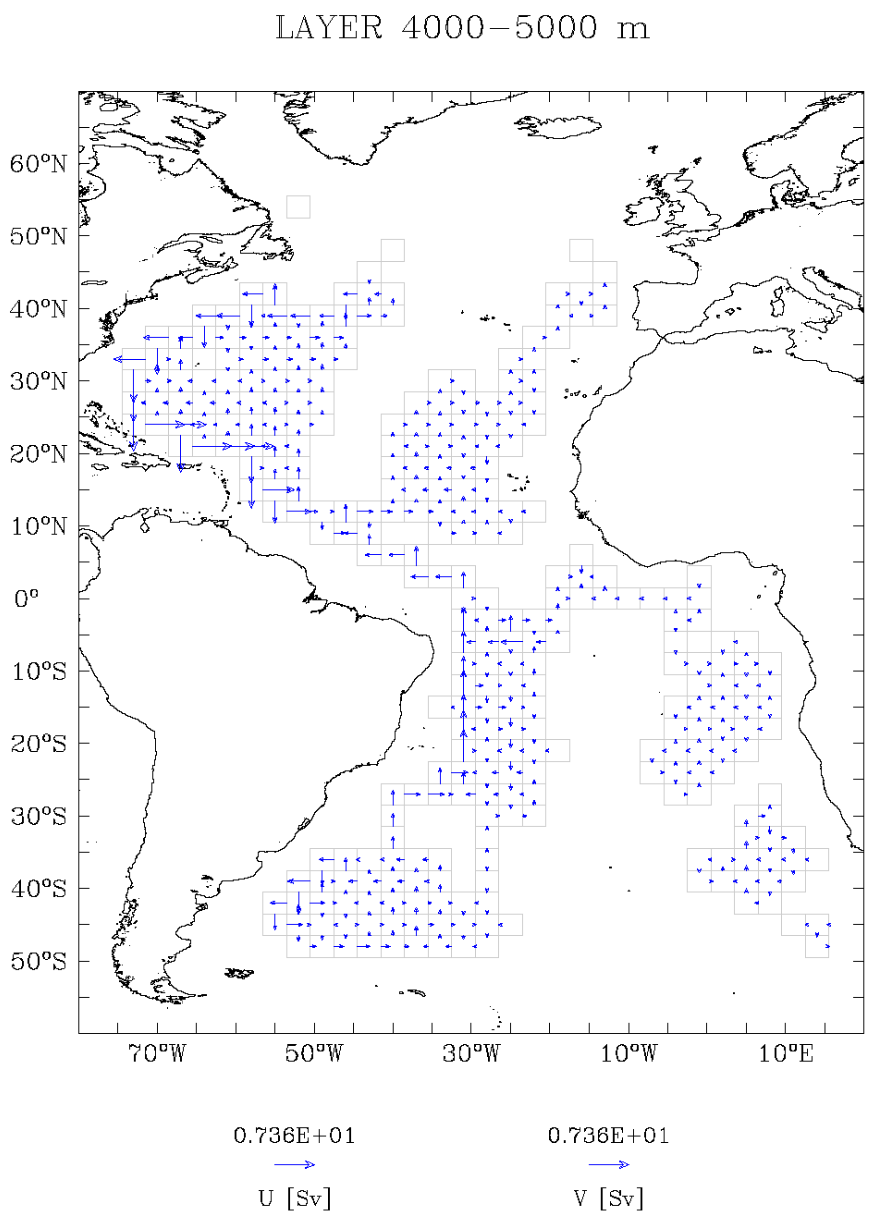
$$\tau \pm \sigma_\tau = 49 \pm 6 \text{ yr}$$

ESTIMATED TRANSPORTS & VENTILATION IN MODERN DEEP ATLANTIC



$$\tau \pm \sigma_\tau = 181 \pm 54 \text{ yr}$$

ESTIMATED TRANSPORTS & VENTILATION IN MODERN DEEP ATLANTIC



$$\tau \pm \sigma_\tau = 346 \pm 48 \text{ yr}$$

NEXT PAGES

- To test H1 (consistency of paleo-$\Delta^{14}C$ data with modern circulation), the $\Delta^{14}C$ transport equation,

$$\frac{\partial C}{\partial t} + \nabla \cdot (\boldsymbol{u}C) = -\lambda C + \epsilon_C, \tag{1}$$

  where $\boldsymbol{u}$ is the modern velocity field, is fitted to the paleo-$\Delta^{14}C$ records using the filter & smoother, and the residuals of the fit are inspected.

- To produce the fit, the following assumptions are made about (i) the initial conditions for $\Delta^{14}C$ and (ii) the equation errors (next two slides)

INITIAL CONDITIONS FOR Δ^{14}C (20 kyr BP)

- Δ^{14}C values

$$\Delta^{14}\mathrm{C}_{ijk}(\mathrm{LGM}) = \Delta^{14}\mathrm{C}_{ijk}(\mathrm{PB}) + \left(\overline{\Delta^{14}\mathrm{C}(\mathrm{LGM})} - \overline{\Delta^{14}\mathrm{C}(\mathrm{PB})}\right)$$

where

$\Delta^{14}\mathrm{C}_{ijk}(\mathrm{PB})$ is Δ^{14}C at grid point (i, j, k) in pre-bomb era (Key et al. 2004)

$\overline{\Delta^{14}\mathrm{C}(\mathrm{LGM})}$ is the mean of Δ^{14}C data for LGM (19-23 kyr BP)

$\overline{\Delta^{14}\mathrm{C}(\mathrm{PB})}$ is the mean of Δ^{14}C data in pre-bomb era

- Δ^{14}C errors

$$\sigma[\Delta^{14}\mathrm{C}_{ijk}(\mathrm{LGM})] = \sigma\left[\Delta^{14}\mathrm{C}(\mathrm{LGM})\right] = \text{std dev of } \Delta^{14}\text{C data for LGM}$$

INITIAL CONDITIONS FOR $\Delta^{14}C$ & EQUATION ERRORS

- Initial conditions (at 20 kyr BP)

$\hat{\boldsymbol{x}}_0(+)$: state estimate including $\Delta^{14}\mathrm{C(LGM)}$ values

$\boldsymbol{P}_0(+)$: error covariance matrix for $\hat{\boldsymbol{x}}_0(+)$:

$$\boldsymbol{P}_0(+) = \sigma^2\left[\Delta^{14}\mathrm{C(LGM)}\right]\mathbf{I}$$

identity matrix

- Equation errors

$\boldsymbol{Q}_i$: error covariance matrix for equation errors ϵ_C and ϵ_B:

$$\boldsymbol{Q}_i = \boldsymbol{Q} = \sigma^2[\nabla \cdot (\boldsymbol{u}C)](\Delta t)^2\ \mathbf{I}$$

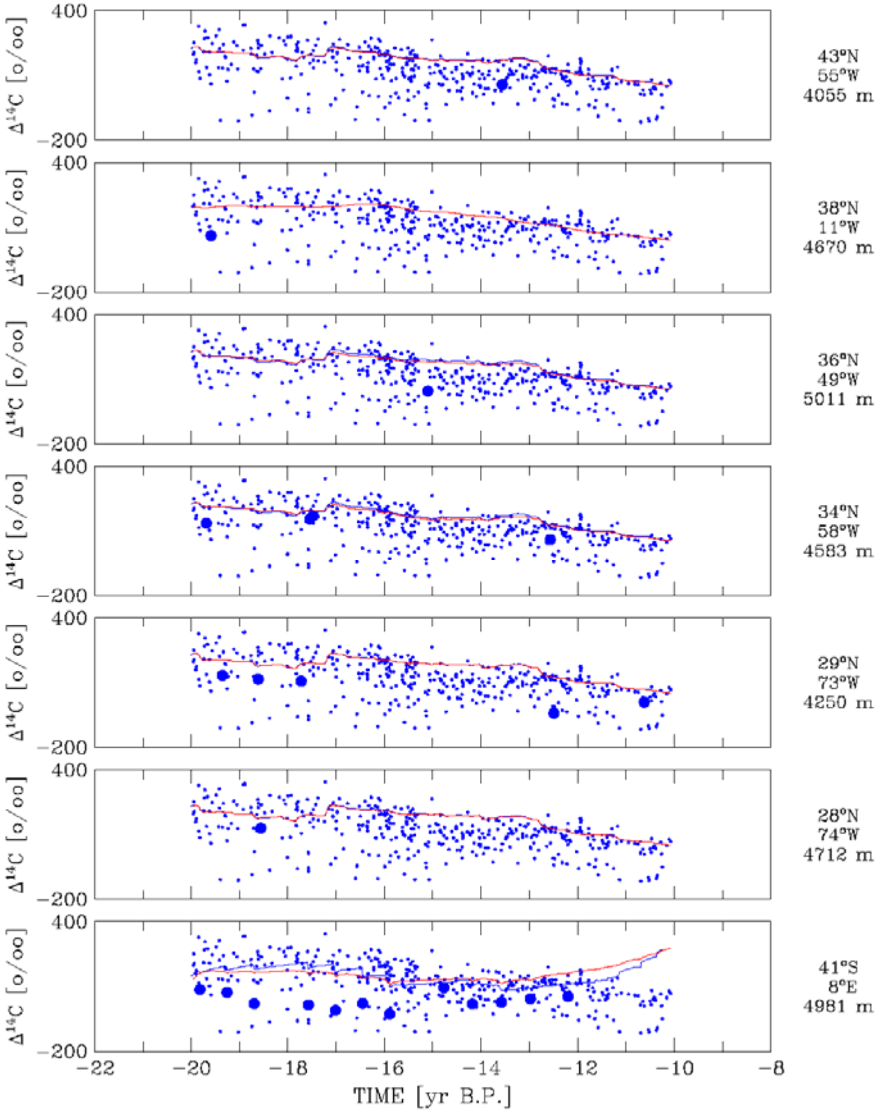
identity matrix

where - $\sigma^2[\nabla \cdot (\boldsymbol{u}C)]$ is the variance of ^{14}C transport divergence in modern ocean
- Δt is the time step of integration

NEXT PAGES

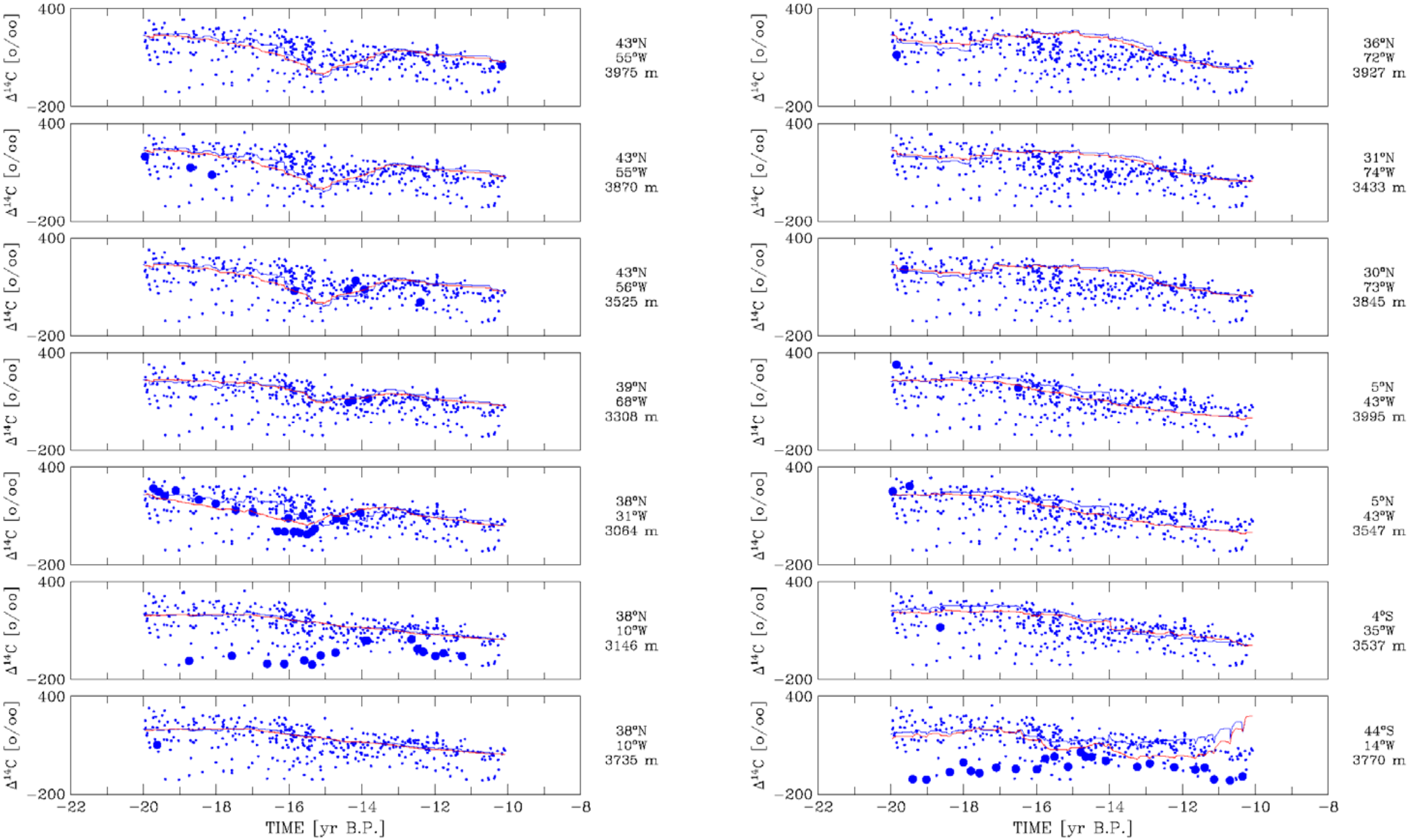
The next pages compare the time series of $\Delta^{14}C$ obtained from the filter and smoother under H1 with the paleo-$\Delta^{14}C$ records in five different layers in the deep Atlantic.

$\Delta^{14}C$ between 4000 – 5000 m

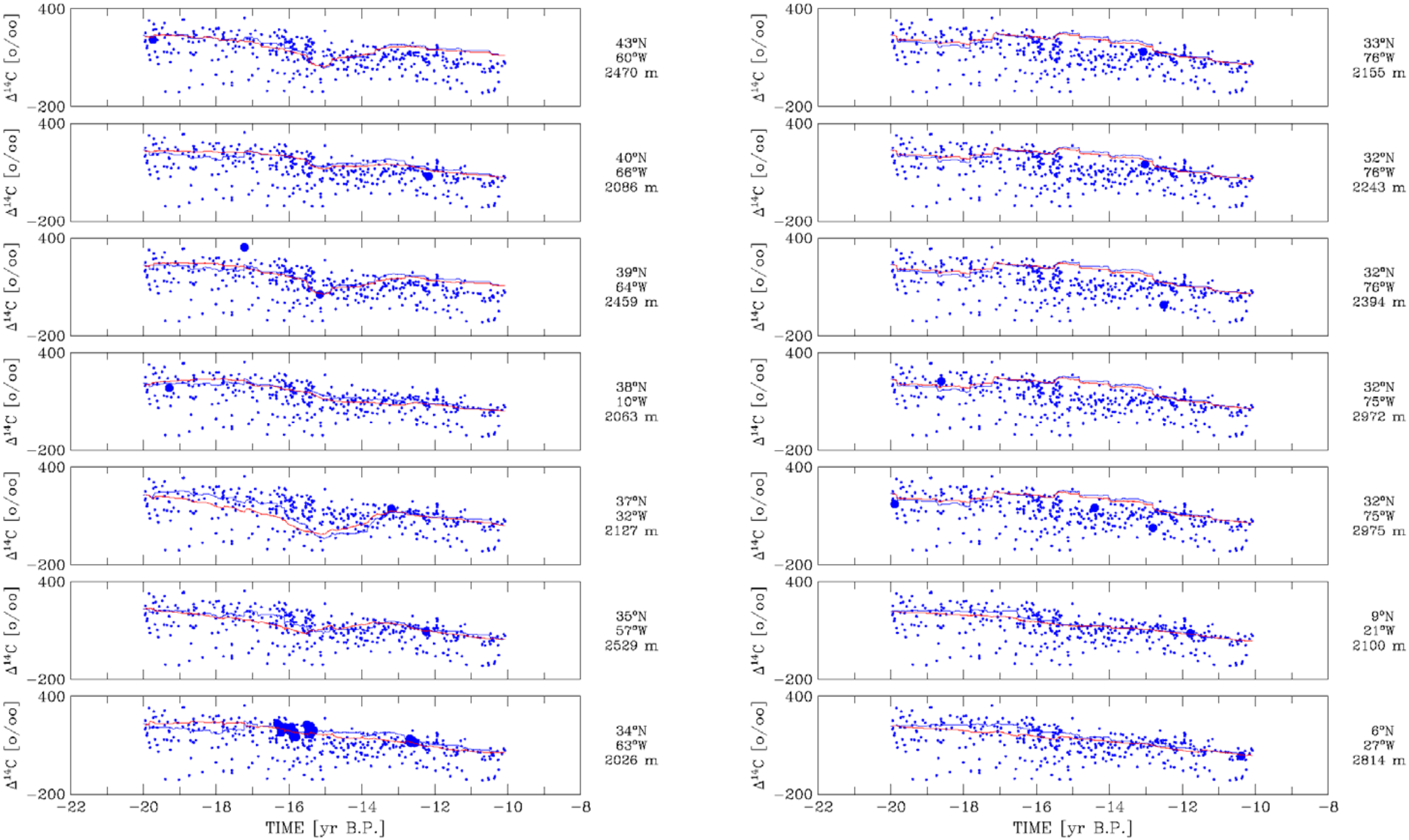


- Paleo-$\Delta^{14}C$ data (at core location)
- Paleo-$\Delta^{14}C$ data (at all locations)
- Filter $\Delta^{14}C$
- Smoother $\Delta^{14}C$

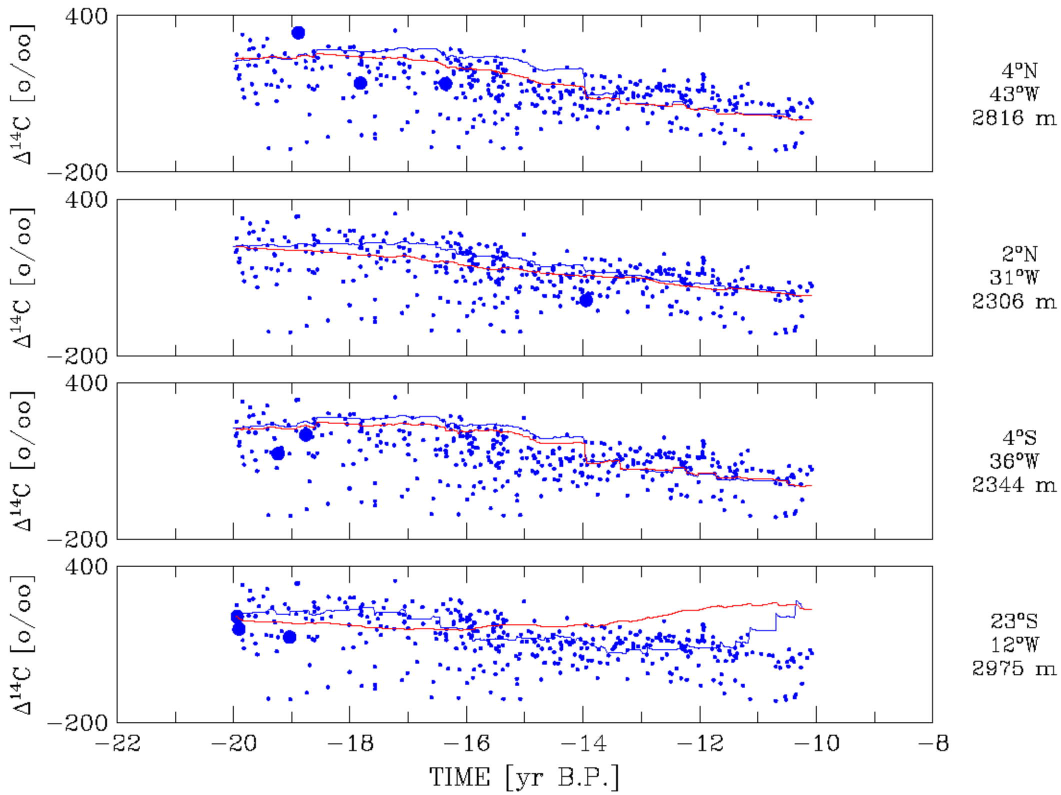
$\Delta^{14}C$ between 3000 – 4000 m



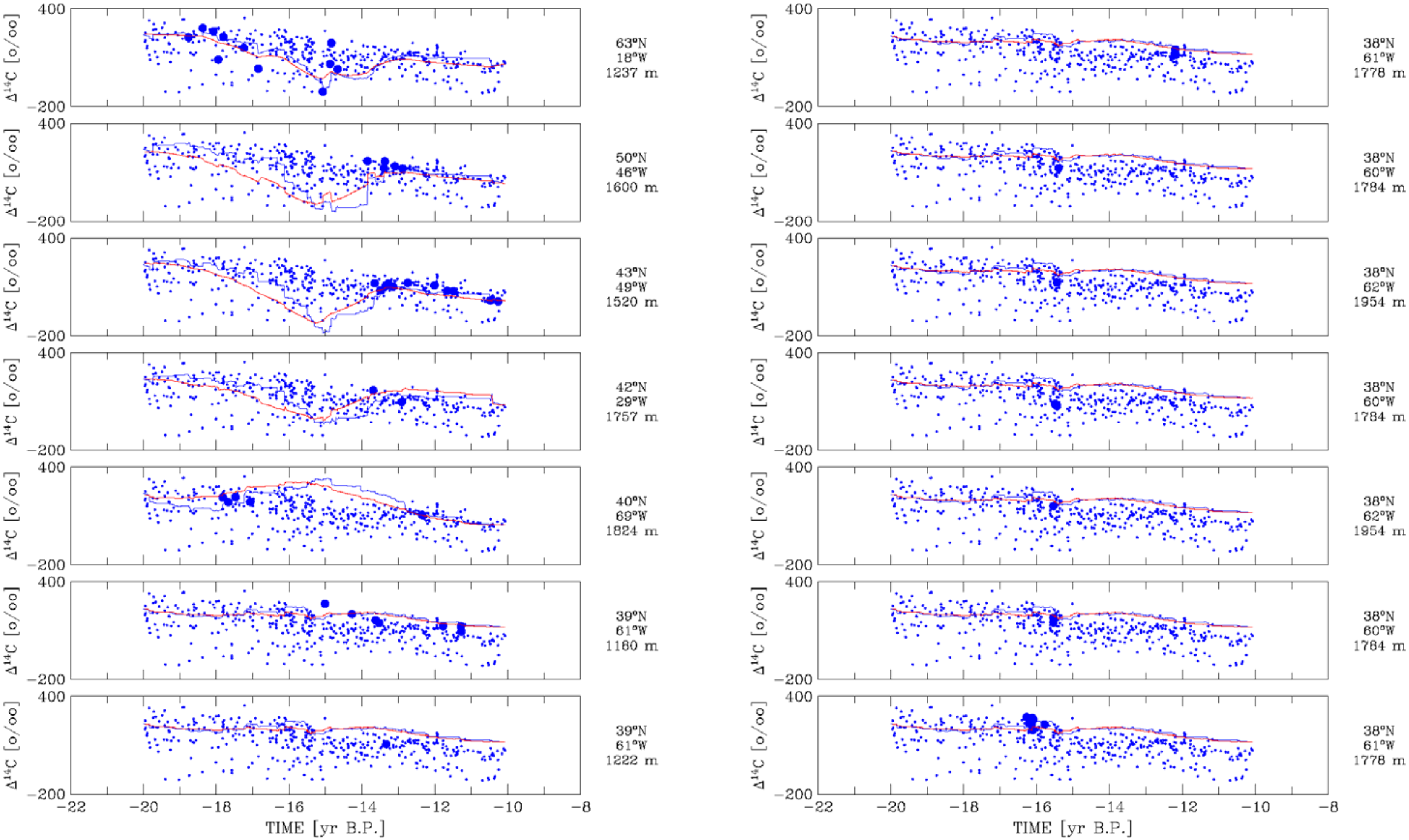
$\Delta^{14}C$ between 2000 – 3000 m



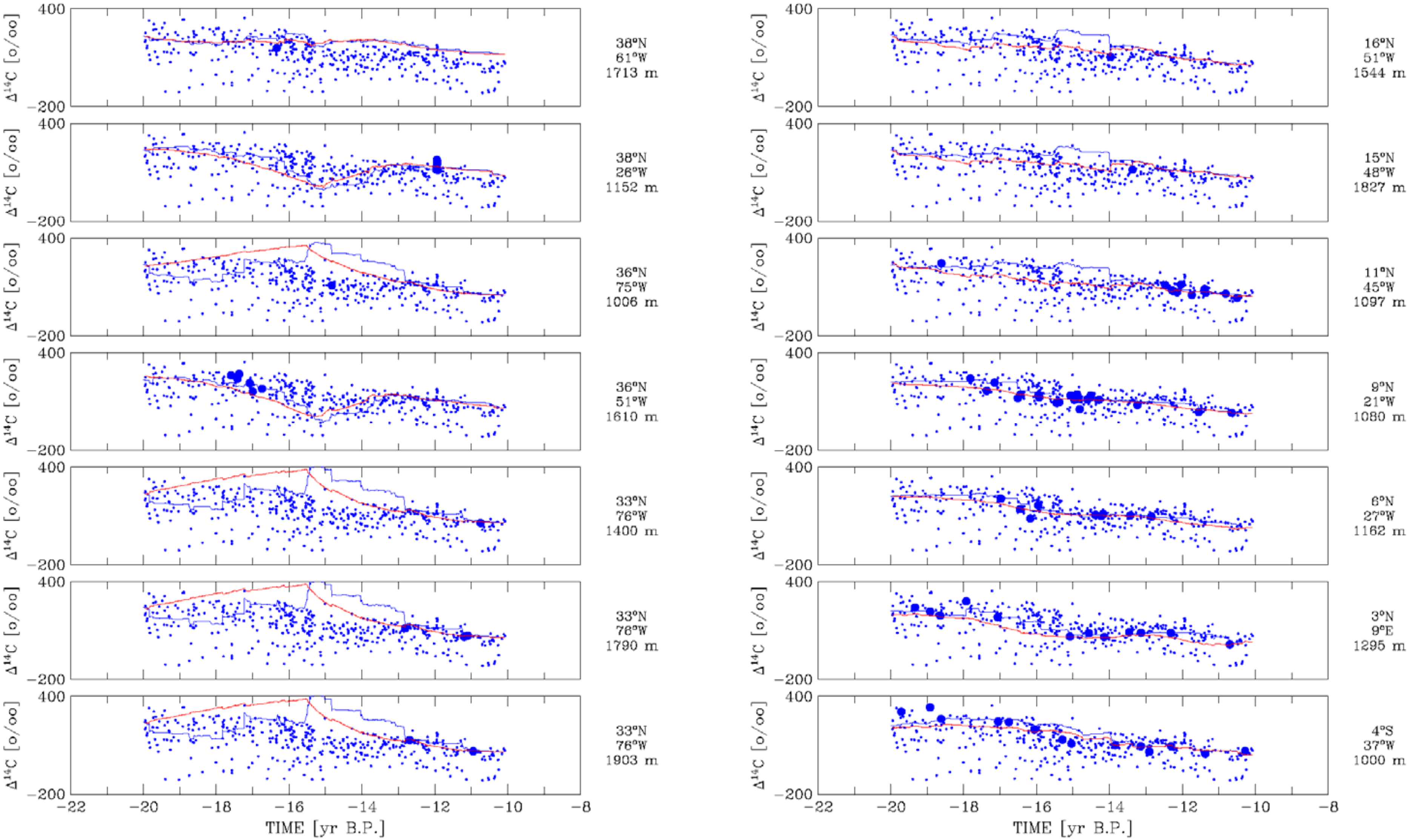
$\Delta^{14}C$ between 2000 – 3000 m



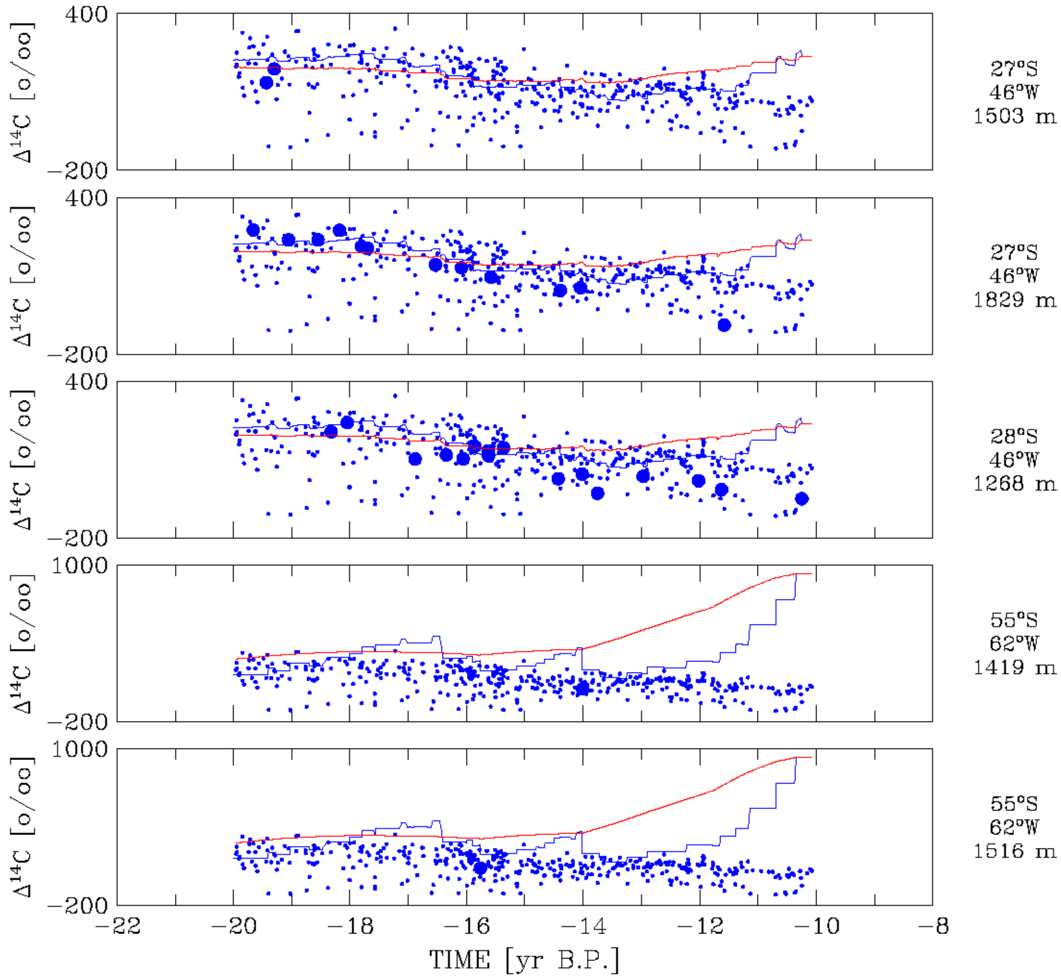
$\Delta^{14}C$ between 1000 – 2000 m



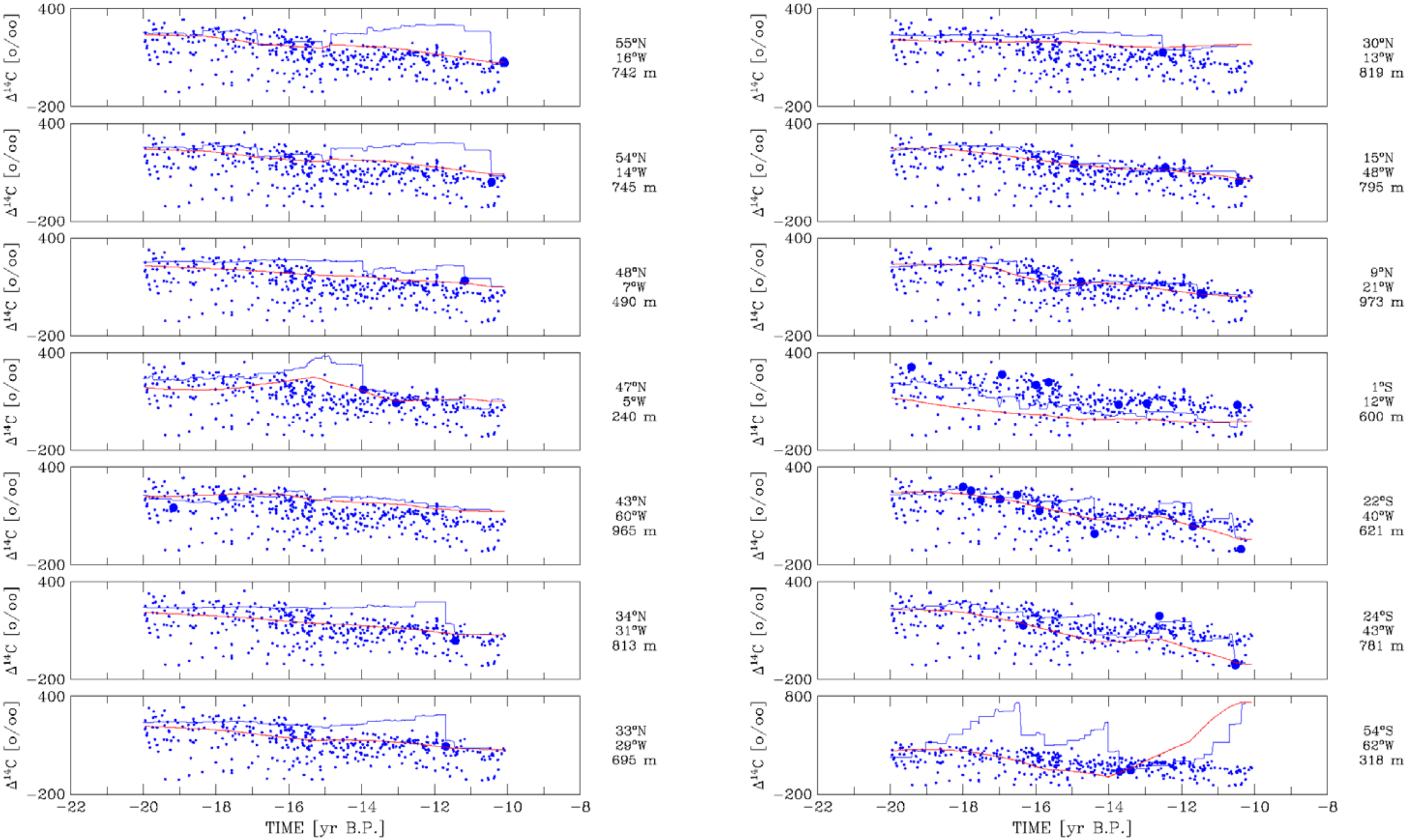
$\Delta^{14}C$ between 1000 – 2000 m



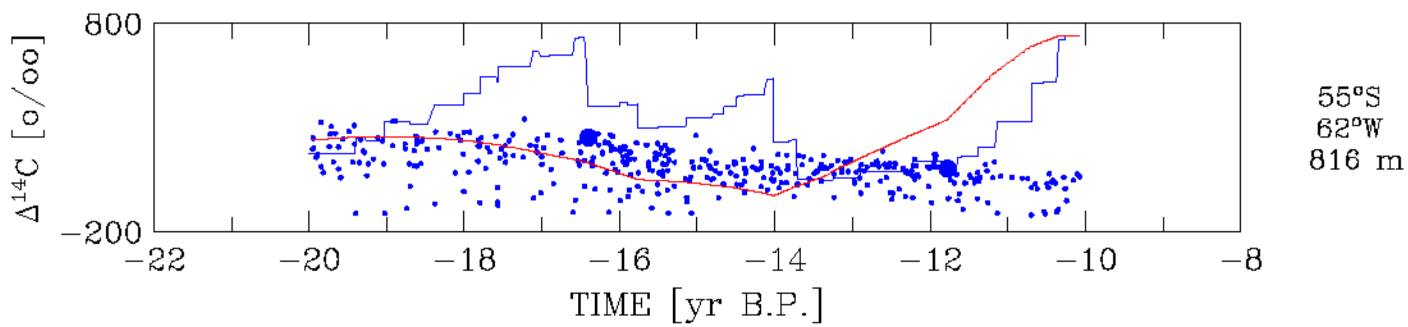
$\Delta^{14}C$ between 1000 – 2000 m



$\Delta^{14}C$ between 0 – 1000 m

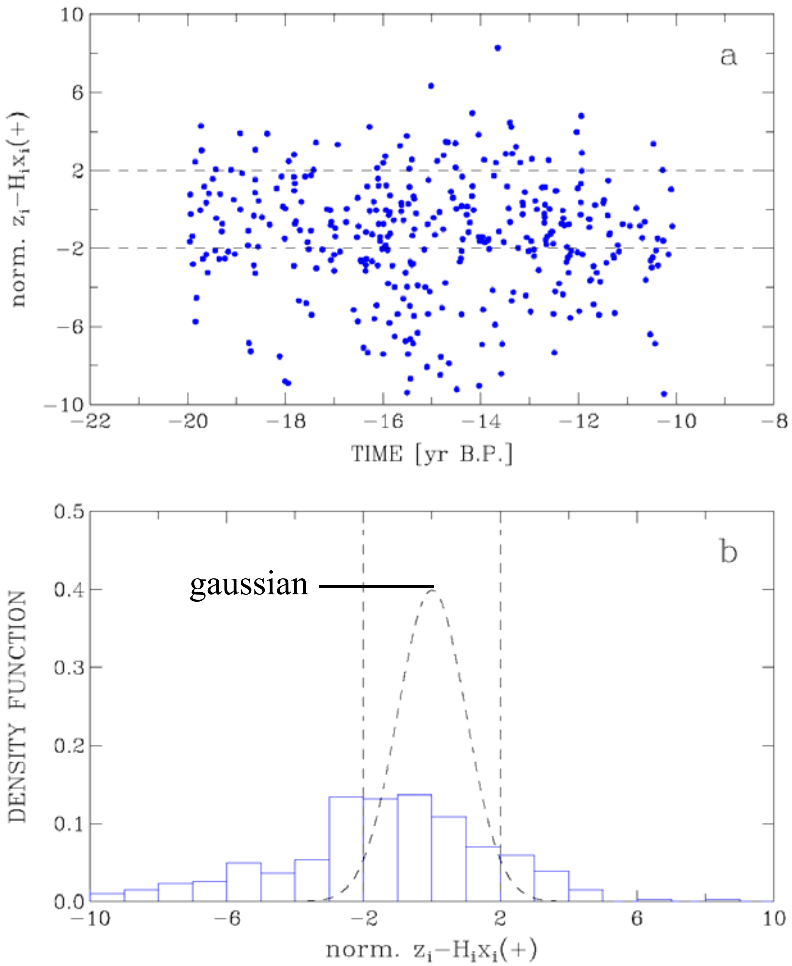


$\Delta^{14}C$ between 0 – 1000 m

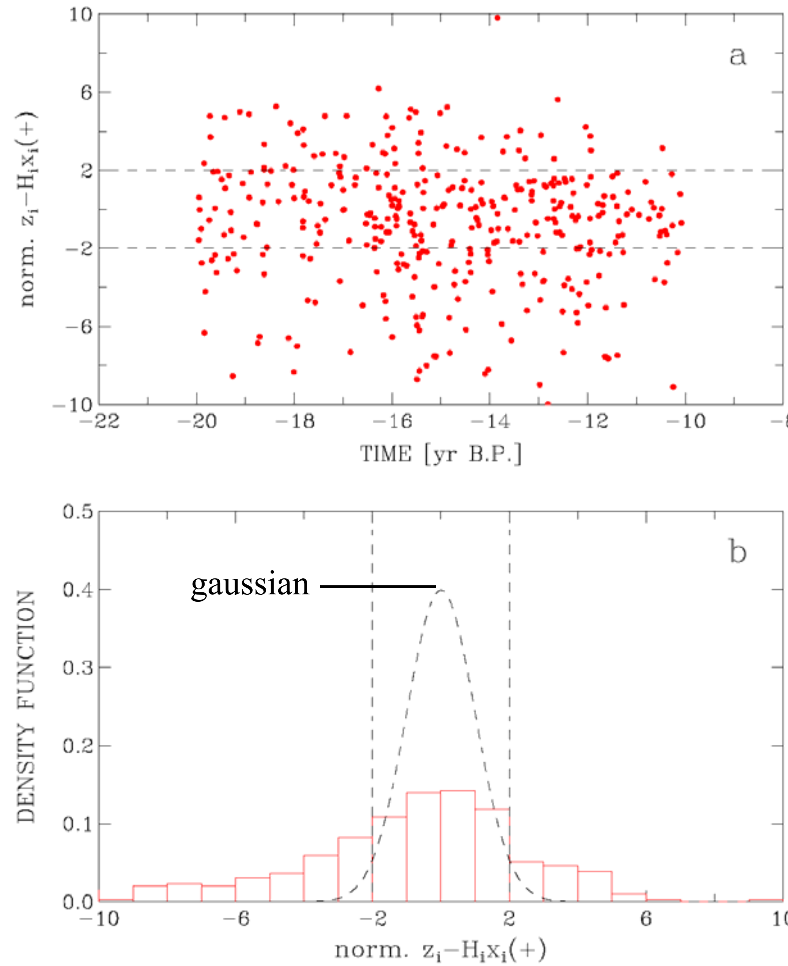


$\Delta^{14}C$ RESIDUALS (normalized to $\Delta^{14}C$ errors) UNDER H1

filter



smoother



→ 55% (49%) of filter (smoother) residuals exceed 2 std dev of paleo-$\Delta^{14}C$ data errors

CONCLUSIONS

- An estimate of the abyssal circulation in the modern Atlantic Ocean is obtained from the quantitative combination of a hydrographic climatology, observational estimates of volume transport, and dynamical constraints.

- According to this estimate, the ventilation time scale increases with increasing depth, amounting to 29 ± 2 yr between 1000 – 2000 m, 49 ± 6 yr between 2000 – 3000 m, 181 ± 54 yr between 3000 – 4000 m, and 346 ± 48 yr between 4000 – 5000 m.

- A preliminary analysis of paleo-Δ^{14}C data for the interval 10-20 kyr BP, which considers uncertainties in the paleo-Δ^{14}C data as well as in Δ^{14}C transport (e.g., mixing), shows that about half of these data are not consistent with our modern circulation estimate, providing support to previous inferences that ventilation rates in the deglacial deep Atlantic were different from modern ones.

- Future work: Examine effects of initial conditions & error assumptions, estimate ventilation changes that would lead to a better fit to paleo-Δ^{14}C records, …

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