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An Overview of Adjoint Modeling

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ECCO Summer School 2025

From Monday

What is an Adjoint Model? (1/2)

From Monday

Adjoint is a transformation used in studying mathematical relationships.

Given a model $\boldsymbol{a} = \mathcal{F}(\boldsymbol{x})$ and "cost" $J \equiv J(\boldsymbol{a})$, what is $\dfrac{\partial J}{\partial \boldsymbol{x}}$?

Given the adjoint $\hat{\boldsymbol{x}} = \hat{\mathcal{F}}(\hat{\boldsymbol{a}})$ and $\hat{\boldsymbol{a}} \equiv \dfrac{\partial J}{\partial \boldsymbol{a}}$, then $\hat{\boldsymbol{x}} = \dfrac{\partial J}{\partial \boldsymbol{x}}$.

Adjoint Method (aka 4D-Var)

Minimize model-data differences J by adjusting the model's controls $\boldsymbol{x}$ using gradients $\dfrac{\partial J}{\partial \boldsymbol{x}}$ computed by the model's adjoint.

Example Computing Gradients (1/2)

Given a model $\boldsymbol{a} = \mathcal{F}(\boldsymbol{x})$ and "cost" $J \equiv J(\boldsymbol{a})$, what is $\dfrac{\partial J}{\partial \boldsymbol{x}}$?

Given the adjoint $\hat{\boldsymbol{x}} = \hat{\mathcal{F}}(\hat{\boldsymbol{a}})$ and $\hat{\boldsymbol{a}} \equiv \dfrac{\partial J}{\partial \boldsymbol{a}}$, then $\hat{\boldsymbol{x}} = \dfrac{\partial J}{\partial \boldsymbol{x}}$.

Example Computing Gradients (1/2)

Given a model $\boldsymbol{a} = \mathcal{F}(\boldsymbol{x})$ and "cost" $J \equiv J(\boldsymbol{a})$, what is $\dfrac{\partial J}{\partial \boldsymbol{x}}$?

Forward Model $\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 & -2 & 3 \\ 4 & 0 & -5 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ $\quad J = \begin{pmatrix} 6 & -7 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$

How? $\mathbf{a} = \mathbf{A}\mathbf{x} \quad J = \mathbf{c}^T\mathbf{a}$ ⇒ $\dfrac{\partial J}{\partial \mathbf{x}} \approx \dfrac{J(\mathbf{a}[\mathbf{x}+\delta\mathbf{x}]) - J(\mathbf{a}[\mathbf{x}])}{\delta\mathbf{x}} \approx \dfrac{\mathbf{c}^T\mathbf{A}\delta\mathbf{x}}{\delta\mathbf{x}}$

$$\frac{\partial J}{\partial x}: \quad \begin{pmatrix} 1 \\ 4 \end{pmatrix} = \begin{pmatrix} 1 & -2 & 3 \\ 4 & 0 & -5 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad \frac{\partial J}{\partial x} = \begin{pmatrix} 6 & -7 \end{pmatrix} \begin{pmatrix} 1 \\ 4 \end{pmatrix} = -22$$

$$\frac{\partial J}{\partial y}: \quad \begin{pmatrix} -2 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & -2 & 3 \\ 4 & 0 & -5 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad \frac{\partial J}{\partial y} = \begin{pmatrix} 6 & -7 \end{pmatrix} \begin{pmatrix} -2 \\ 0 \end{pmatrix} = -12$$

$$\frac{\partial J}{\partial z}: \quad \begin{pmatrix} 3 \\ -5 \end{pmatrix} = \begin{pmatrix} 1 & -2 & 3 \\ 4 & 0 & -5 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad \frac{\partial J}{\partial z} = \begin{pmatrix} 6 & -7 \end{pmatrix} \begin{pmatrix} 3 \\ -5 \end{pmatrix} = 53$$

Example Computing Gradients (2/2)

Given the adjoint $\hat{\boldsymbol{x}} = \hat{\mathcal{F}}(\hat{\boldsymbol{a}})$ and $\hat{\boldsymbol{a}} \equiv \dfrac{\partial J}{\partial \boldsymbol{a}}$, then $\hat{\boldsymbol{x}} = \dfrac{\partial J}{\partial \boldsymbol{x}}$.

Forward Model $\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 & -2 & 3 \\ 4 & 0 & -5 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$ $\quad J = (6 \quad -7) \begin{pmatrix} a \\ b \end{pmatrix}$

Adjoint Model $\begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix} = \begin{pmatrix} 1 & 4 \\ -2 & 0 \\ 3 & -5 \end{pmatrix} \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix}$ $\quad \begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} = \begin{pmatrix} \partial J/\partial a \\ \partial J/\partial x \end{pmatrix} = \begin{pmatrix} 6 \\ -7 \end{pmatrix}$

$$\begin{pmatrix} \partial J/\partial x \\ \partial J/\partial y \\ \partial J/\partial z \end{pmatrix} = \begin{pmatrix} 1 & 4 \\ -2 & 0 \\ 3 & -5 \end{pmatrix} \begin{pmatrix} 6 \\ -7 \end{pmatrix} = \begin{pmatrix} -22 \\ -12 \\ 53 \end{pmatrix}$$

Why so? Given $\mathbf{a} = \mathbf{A}\mathbf{x}$ $\quad J = \mathbf{c}^T \mathbf{a}$ $\Rightarrow$ $\dfrac{\partial J}{\partial \mathbf{x}} = \dfrac{\partial \mathbf{a}}{\partial \mathbf{x}} \dfrac{\partial J}{\partial \mathbf{a}} = \mathbf{A}^T \mathbf{c}$

Example Computing Gradients (2/2)

From Yesterday

... adjoint $\hat{\boldsymbol{x}} = \hat{\mathcal{F}}(\hat{\boldsymbol{a}})$ and $\hat{\boldsymbol{a}} \equiv \dfrac{\partial J}{\partial \boldsymbol{a}}$, then $\hat{\boldsymbol{x}} = \dfrac{\partial J}{\partial \boldsymbol{x}}$.

Least-Squares Estimate (3/4)

To minimizes $\boxed{J = (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x})^T \mathbf{R}^{-1} (\hat{\mathbf{y}} - \mathbf{H}\mathbf{x}) + \mathbf{x}^T \mathbf{P}^{-1} \mathbf{x}}$

Solve $\dfrac{\partial J}{\partial \mathbf{x}} = \mathbf{0}$

Basic notation of vector differentiation

$$\frac{\partial s}{\partial \mathbf{x}} \equiv \left(\frac{\partial s}{\partial x_1} \quad \cdots \quad \frac{\partial s}{\partial x_N} \right)^T \Rightarrow \frac{\partial (\boldsymbol{q}^T \mathbf{x})}{\partial \mathbf{x}} = \frac{\partial (\mathbf{x}^T \boldsymbol{q})}{\partial \mathbf{x}} = \boldsymbol{q}$$

$$\frac{\partial \boldsymbol{q}}{\partial \mathbf{x}} \equiv \begin{pmatrix} \frac{\partial q_1}{\partial x_1} & \cdots & \frac{\partial q_M}{\partial x_1} \\ \vdots & \cdots & \vdots \\ \frac{\partial q_1}{\partial x_N} & \cdots & \frac{\partial q_M}{\partial x_N} \end{pmatrix} \Rightarrow \frac{\partial (\mathbf{B}\mathbf{x})}{\partial \mathbf{x}} = \mathbf{B}^T \quad \frac{\partial (\mathbf{x}^T \mathbf{B})}{\partial \mathbf{x}} = \mathbf{B}$$

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$$J = (6 \quad -7) \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\begin{pmatrix} \hat{a} \\ \hat{b} \end{pmatrix} = \begin{pmatrix} \partial J / \partial a \\ \partial J / \partial x \end{pmatrix} = \begin{pmatrix} 6 \\ -7 \end{pmatrix}$$

$$\ldots \begin{pmatrix} 6 \\ -7 \end{pmatrix} = \begin{pmatrix} -22 \\ -12 \\ 53 \end{pmatrix}$$

Why so? Given $\mathbf{a} = \mathbf{A}\mathbf{x}$ $\quad J = \mathbf{c}^T \mathbf{a}$ $\Rightarrow$ $\dfrac{\partial J}{\partial \mathbf{x}} = \dfrac{\partial \mathbf{a}}{\partial \mathbf{x}} \dfrac{\partial J}{\partial \mathbf{a}} = \mathbf{A}^T \mathbf{c}$

Adjoint of Time-Evolving Model

$$\mathbf{x}_{t+1} = \mathbf{A}_t \mathbf{x}_t + \mathbf{G}_t \mathbf{u}_t \qquad J = \mathbf{w}^T \mathbf{x}_T$$

$$\frac{\partial J}{\partial \mathbf{x}_{T-N}} = \frac{\partial \mathbf{x}_{T-N+1}}{\partial \mathbf{x}_{T-N}} \frac{\partial \mathbf{x}_{T-N+2}}{\partial \mathbf{x}_{T-N+1}} \cdots \frac{\partial \mathbf{x}_{T}}{\partial \mathbf{x}_{T-1}} \frac{\partial J}{\partial \mathbf{x}_{T}}$$

$$= \mathbf{A}_{T-N}{}^T \mathbf{A}_{T-N+1}{}^T \ldots \mathbf{A}_{T-1}{}^T \mathbf{w}$$

$$\frac{\partial J}{\partial \mathbf{u}_{T-N}} = \frac{\partial \mathbf{x}_{T-N+1}}{\partial \mathbf{u}_{T-N}} \frac{\partial \mathbf{x}_{T-N+2}}{\partial \mathbf{x}_{T-N+1}} \cdots \frac{\partial \mathbf{x}_{T}}{\partial \mathbf{x}_{T-1}} \frac{\partial J}{\partial \mathbf{x}_{T}}$$

$$= \mathbf{G}_{T-N}{}^T \mathbf{A}_{T-N+1}{}^T \ldots \mathbf{A}_{T-1}{}^T \mathbf{w}$$

What Good is an Adjoint Model?

1) Circulation Pathways

2) Causation

Circulation Pathway (1/9)

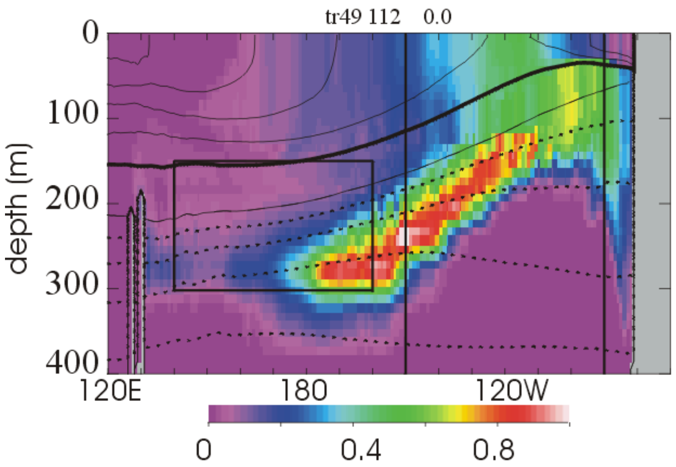
Passive tracers describe where a tracer-tagged water goes, i.e., its fate.

$$\frac{\partial c}{\partial t} = -\mathbf{u} \cdot \boldsymbol{\nabla} c + \boldsymbol{\nabla} \cdot (\kappa \boldsymbol{\nabla} c)$$

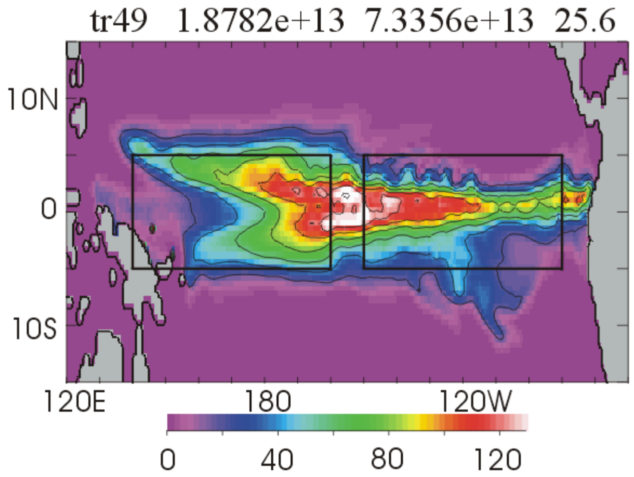
Passive Tracer
@12/31/2020

Initialized 1/1/2020 uniform to 1 over 150-300m, 5S-5N, 140E-160W

c along Equator



$\int c\, dz$



Average value of 0.25 over 0-10m, 5S-5N, 150W-90W

Circulation Pathway (2/9)

What is the sensitivity of passive tracer content **c** at location (i,j,k) to tracer distribution in the past?

$$(i,j,k)$$

Objective Function $\quad J = (0 \quad \cdots \quad 0 \quad 1 \quad 0 \quad \cdots \quad 0)^T \mathbf{c}_{\mathrm{T}} = \mathbf{w}^T \ \mathbf{c}_{\mathrm{T}}$

$$\frac{\partial c}{\partial t} = -\mathbf{u} \cdot \boldsymbol{\nabla} c + \boldsymbol{\nabla} \cdot (\kappa \boldsymbol{\nabla} c)$$

Adjoint

$$\frac{\partial J}{\partial \mathbf{c}_t} \equiv \mathbf{c}' \qquad\qquad -\frac{\partial c'}{\partial t} = \ \mathbf{u} \cdot \boldsymbol{\nabla} c' + \boldsymbol{\nabla} \cdot (\kappa \boldsymbol{\nabla} c')$$

$$\frac{\partial J}{\partial \mathbf{c}_{\mathrm{T}}} \equiv \mathbf{c}'_{\mathrm{T}} = \mathbf{w}$$

Circulation Pathway (3/9)

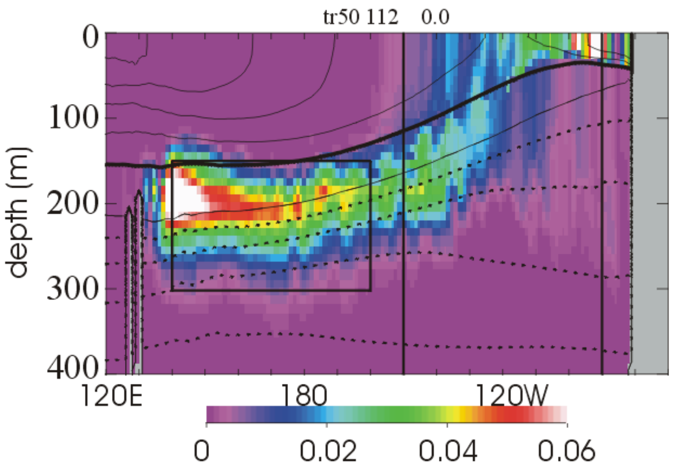
Adjoint passive tracers describe where an adjoint tracer-tagged water comes from, i.e., its origin.

$$-\frac{\partial c'}{\partial t} = \mathbf{u}\cdot\nabla c' + \nabla\cdot(\kappa\nabla c')$$

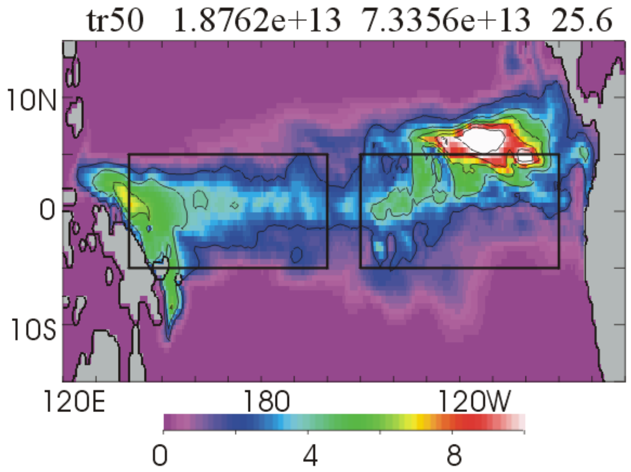
Adjoint Passive Tracer @1/1/2020

Initialized 12/31/2020 uniform to 1 over 0-10m, 5S-5N, 150W-90W

c' along Equator



$\int c'\,dz$



Volumetric fraction over 150-300m, 5S-5N, 140E-160W is 0.25

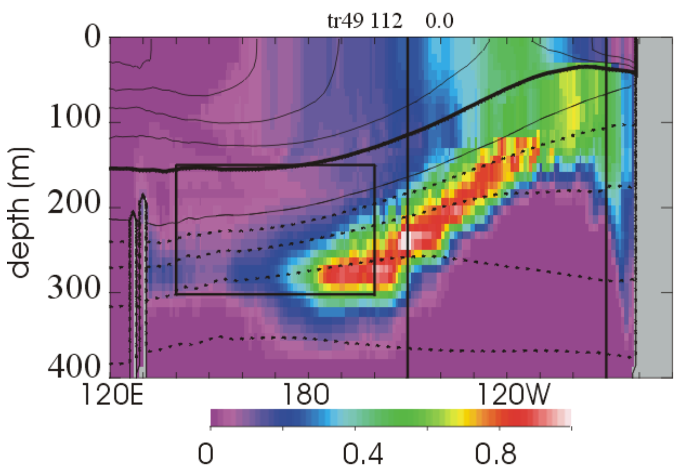
Circulation Pathway (4/9)

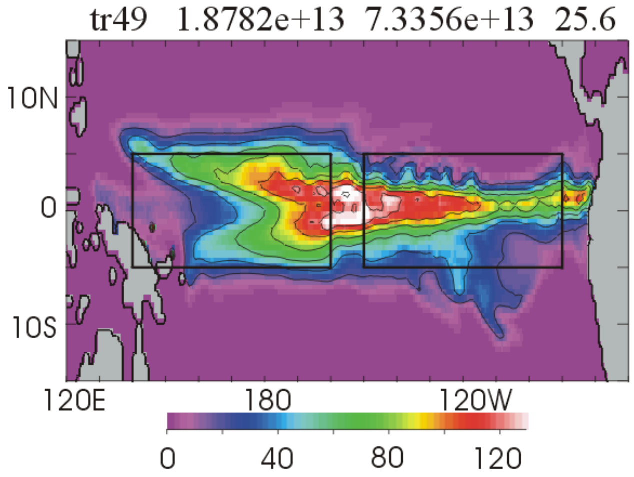
c' along Equator

$\int c' \, dz$

Passive Tracer
12/31/2020

Initialized 1/1/2020
uniform to 1 over
150-300m, 5S-5N,
140E-160W

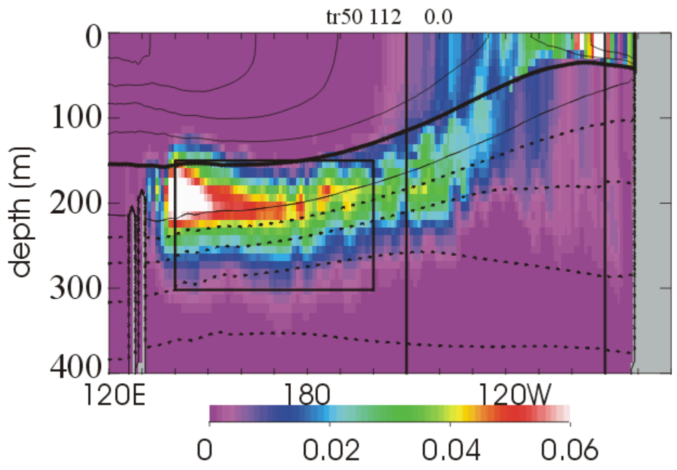


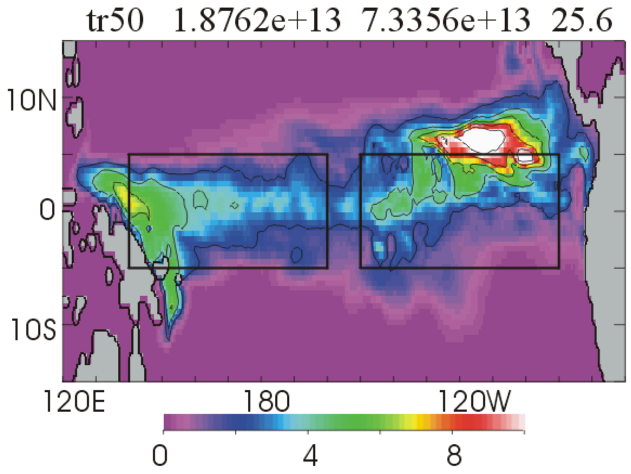


Average value of 0.25
over 0-10m, 5S-5N,
150W-90W

Adjoint Passive Tracer
1/1/2020

Initialized 12/31/2020
uniform to 1 over
0-10m, 5S-5N,
150W-90W



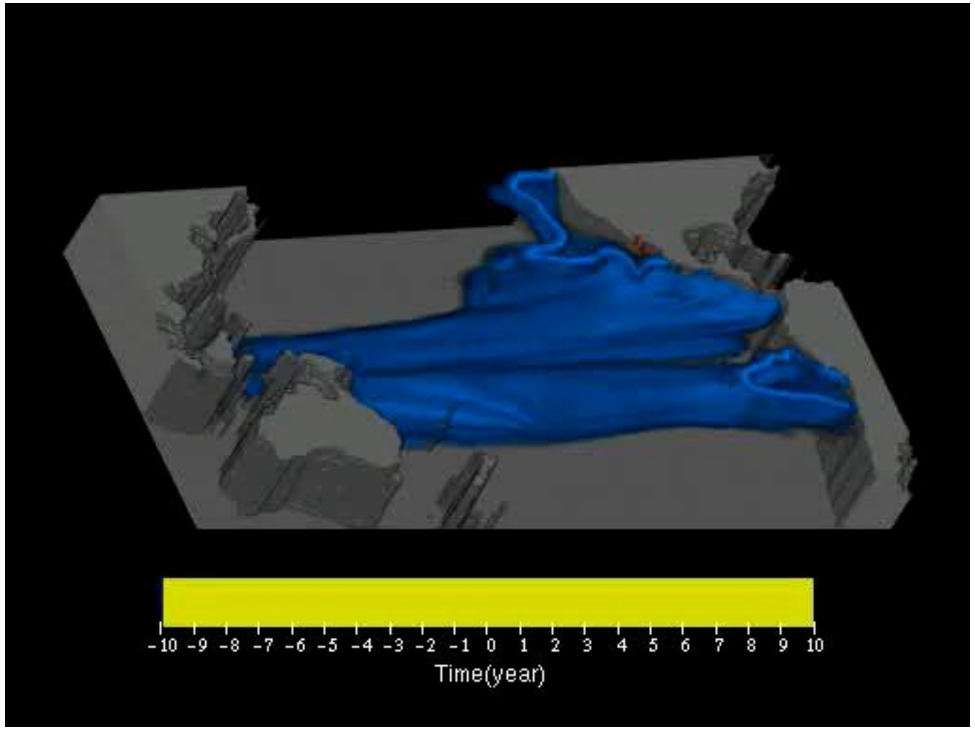


Volumetric fraction
over 150-300m, 5S-5N,
140E-160W
is 0.25

Circulation Pathway (5/9)

Origin and Fate of Niño-3 Water

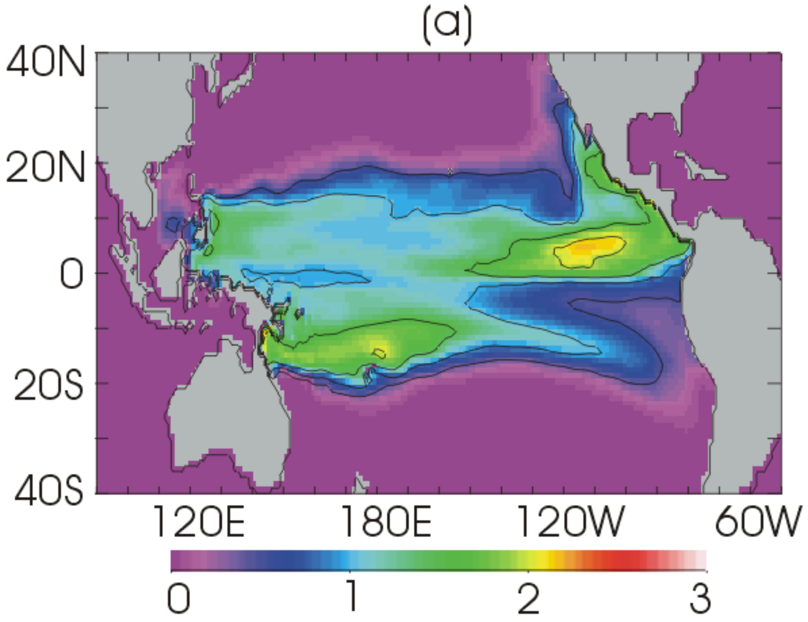
Adjoint (years<0) and forward (years>0) passive tracer simulation of water occupying Niño-3 area (5°S-5°N, 150°W-90°W). Tracer extent shown in blue. Red shows regions of highest concentration.



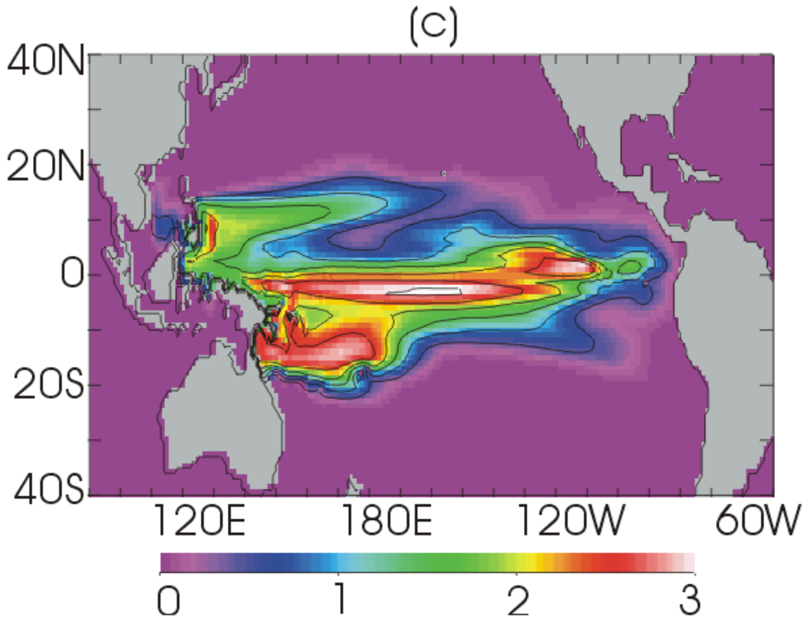
Circulation Pathway (6/9)

"Time-Mean" Circulation

Mean Distribution (t = - 5 years)

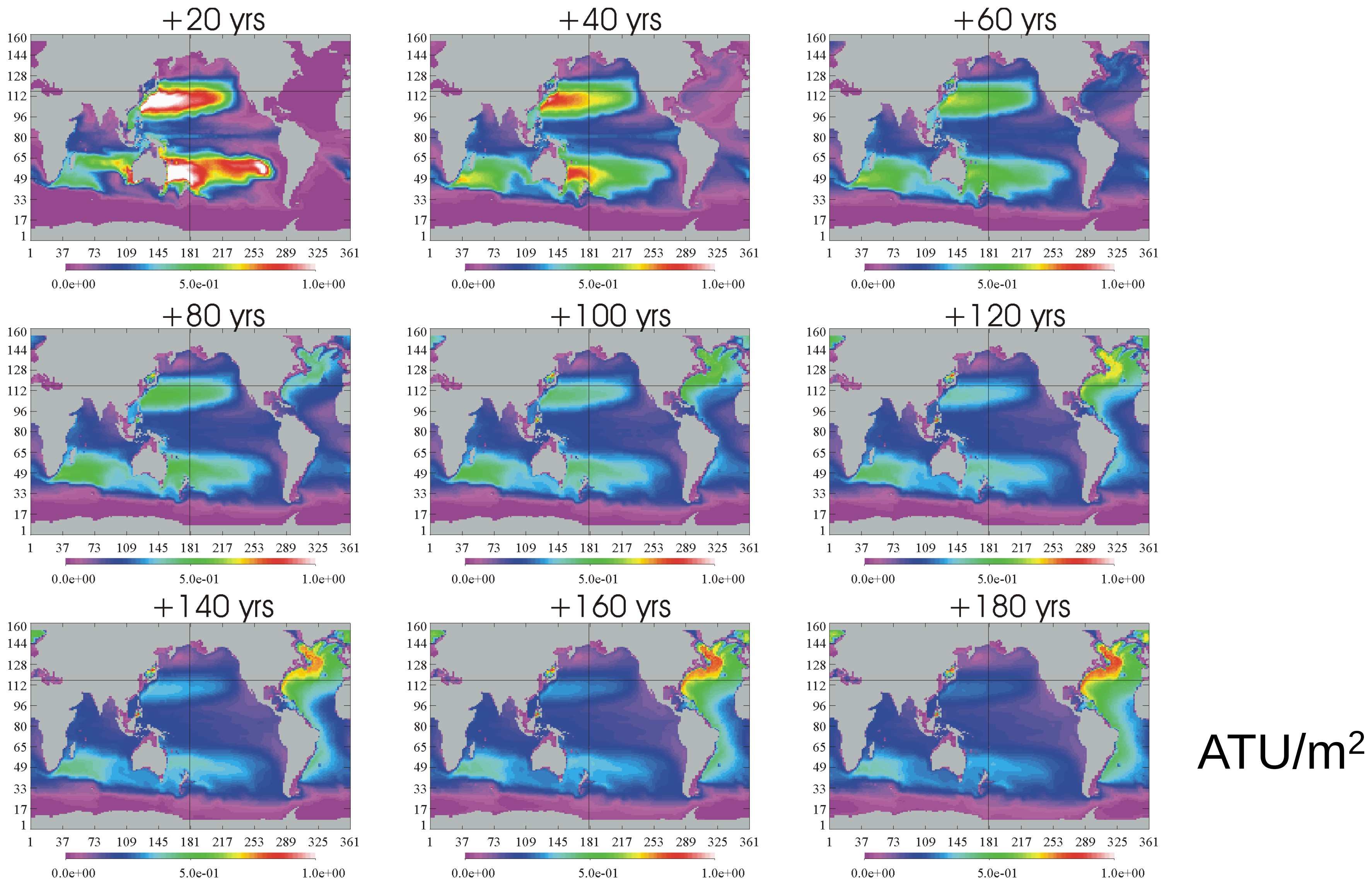


Distribution inferred from mean circulation (t = - 5 years)



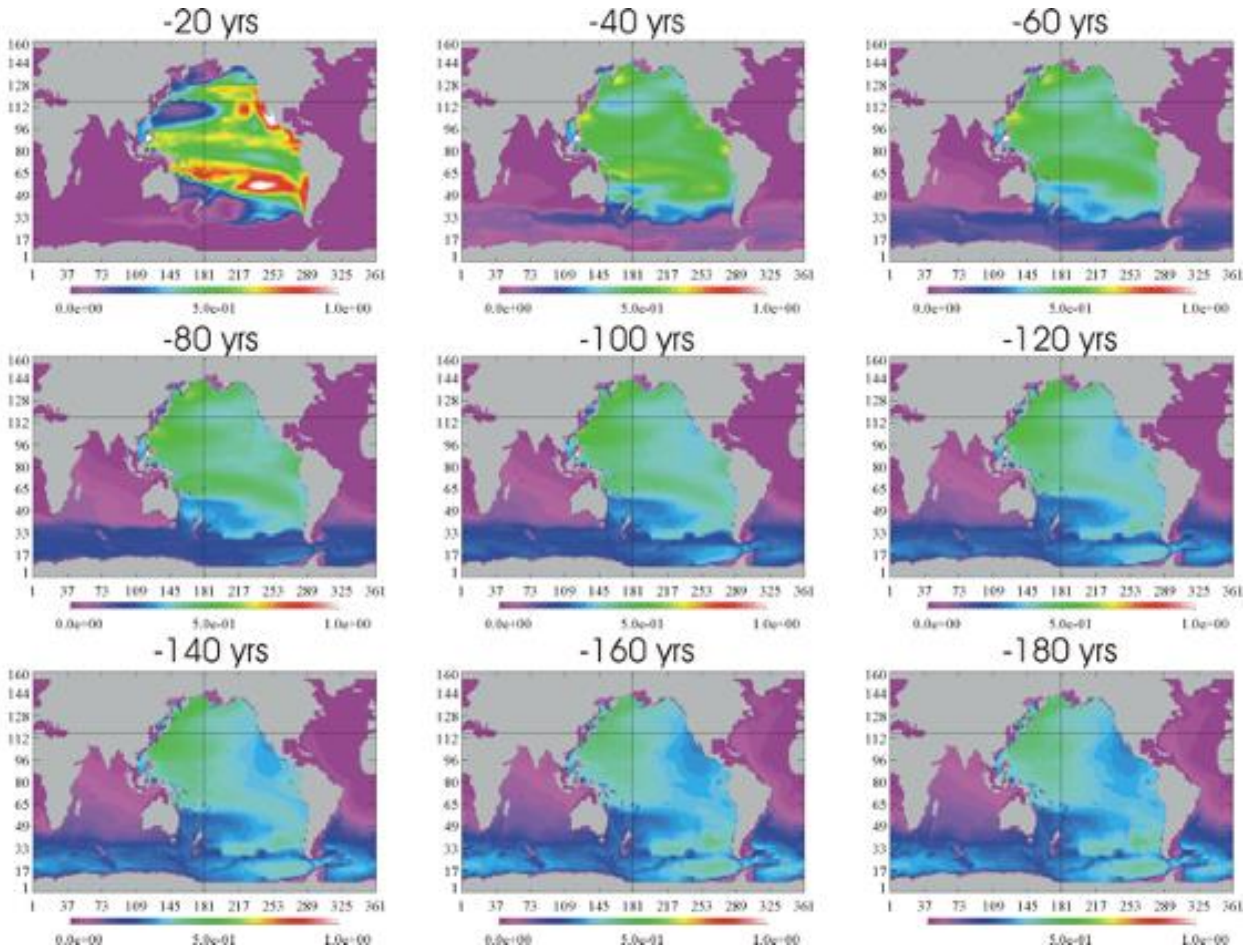
Circulation Pathway (7/9)

Where does the Nino3 water go over 20~180 years?



Circulation Pathway (8/9)

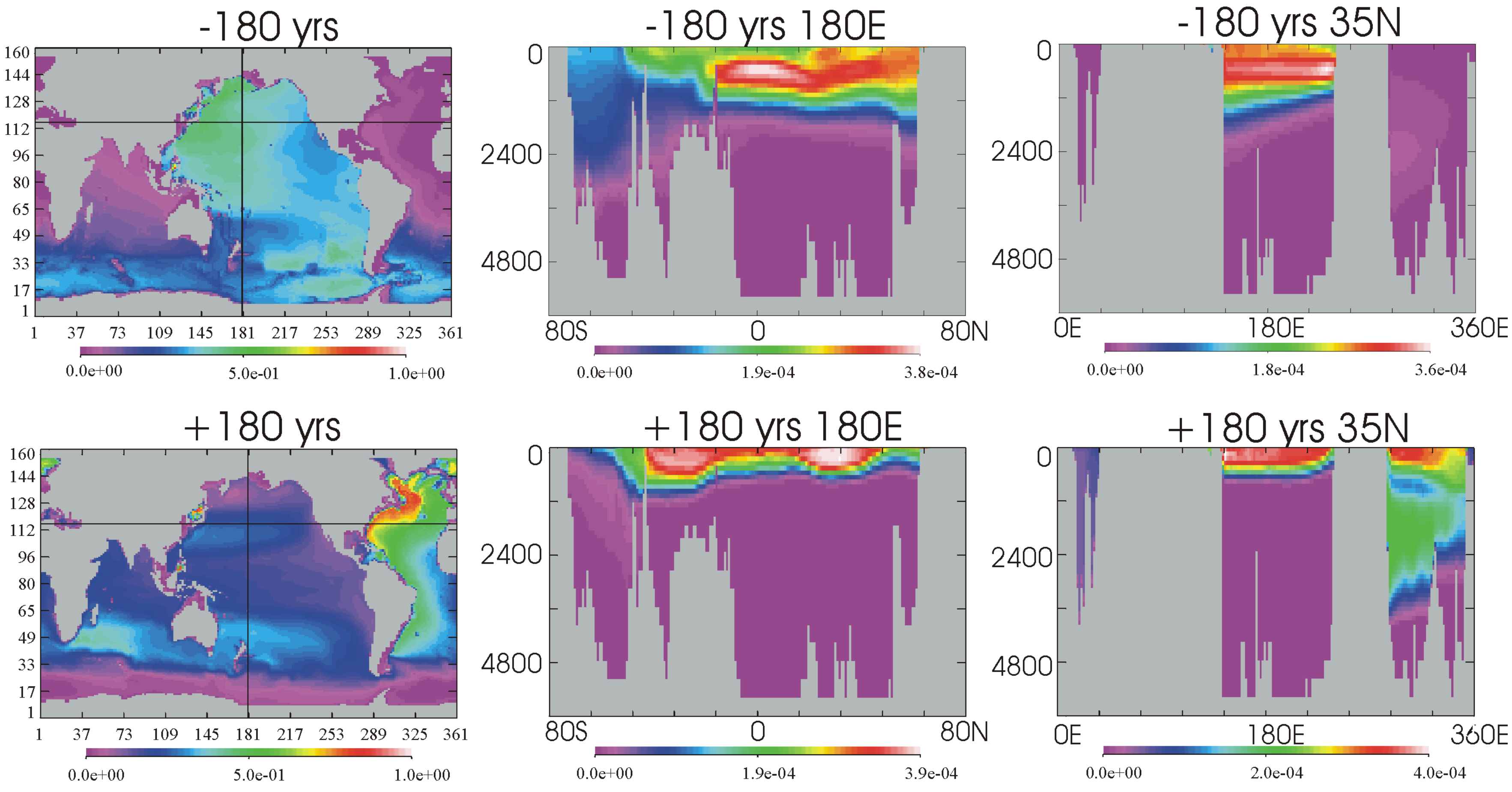
Where was the Nino3 water 20~180 years prior?



ATU/m^2

Circulation Pathway (9/9)

Where from and where to @ ±180 yrs



ATU/m^2 ATU/m^3 ATU/m^3

Example Studies Using Adjoint Passive Tracers

Chhak, K., & di Lorenzo, E. (2007). Decadal variations in the California Current upwelling cells. Geophysical Research Letters, 34(14). doi:10.1029/2007GL030203

Fukumori, I., T. Lee, B. Cheng, and D. Menemenlis, (2004). The origin, pathway, and destination of Nino-3 water estimated by a simulated passive tracer and its adjoint. *J Phys Oceanogr*, **34,** 582-604, doi:10.1175/2515.1.

Gao, S., T. Qu, and I. Fukumori (2011). Effects of mixing on the subduction of South Pacific waters identified by a simulated passive tracer and its adjoint, Dyn. Atmos. Oceans., 54, 45-54, doi:10.1016/J.Dynatmoce.2010.10.002.

Gao, S., T. Qu, and D. Hu (2012), Origin and pathway of the Luzon Undercurrent identified by a simulated adjoint tracer, J. Geophys. Res., 117, C05011, doi:10.1029/2011JC007748.

Nie, X., Gao, S., Wang, F., Chi, J., & Qu, T. (2019). Origins and Pathways of the Pacific Equatorial Undercurrent Identified by a Simulated Adjoint Tracer. Journal of Geophysical Research: Oceans, 124(4), 2331–2347. doi:10.1029/2018JC014212

Qu, T., S. Gao, I. Fukumori, R. A. Fine, and E. J. Lindstrom (2009). Origin and pathway of Equatorial 13°C Water in the Pacific identified by a simulated passive tracer and its adjoint, J. Phys. Oceanogr., 39, 1836-1853, doi:10.1175/2009jpo4045.1

Qu, T., S. Gao, and I. Fukumori (2013). Formation of salinity maximum water and its contribution to the overturning circulation in the North Atlantic as revealed by a global GCM, Journal of Geophysical Research: Oceans, 118(4), 1982-1994, doi:10.1002/jgrc.20152.

Song, H., Miller, A. J., Cornuelle, B. D., & di Lorenzo, E. (2011). Changes in upwelling and its water sources in the California Current System driven by different wind forcing. Dynamics of Atmospheres and Oceans, 52(1), 170–191. doi:10.1016/j.dynatmoce.2011.03.001

Stephenson, D., Müller, S. A., & Sévellec, F. (2020). Tracking water masses using passive-tracer transport in NEMO v3.4 with NEMOTAM: application to North Atlantic Deep Water and North Atlantic Subtropical Mode Water. Geoscientific Model Development, 13(4), 2031–2050. doi:10.5194/gmd-13-2031-2020

Valsala, V., Maksyutov, S., & Murtugudde, R. (2011). Interannual to Interdecadal Variabilities of the Indonesian Throughflow Source Water Pathways in the Pacific Ocean. Journal of Physical Oceanography, 41(10), 1921–1940. doi:10.1175/2011JPO4561.1

Causation (1/9)

Adjoint gradients can help identify causal mechanisms of the dynamic system.

$$\delta J(t) \approx \boxed{\sum_i \sum_{\mathbf{r}} \sum_{\Delta t}} \frac{\partial J(t)}{\partial u_i(\mathbf{r}, t-\Delta t)} \delta u_i(\mathbf{r}, t-\Delta t)$$

$$\approx \sum_i \sum_{\mathbf{r}} \sum_{\Delta t} \frac{\partial J(T)}{\partial u_i(\mathbf{r}, T-\Delta t)} \delta u_i(\mathbf{r}, t-\Delta t)$$

$$\approx \sum_i \sum_{\mathbf{r}} \sum_{\Delta t} \frac{\partial J}{\partial u_i}(\mathbf{r}, \Delta t)\, \delta u_i(\mathbf{r}, t-\Delta t)$$

Quantity of interest at time t.

Type (i), location ($\mathbf{r}$), and lag (Δt) of control

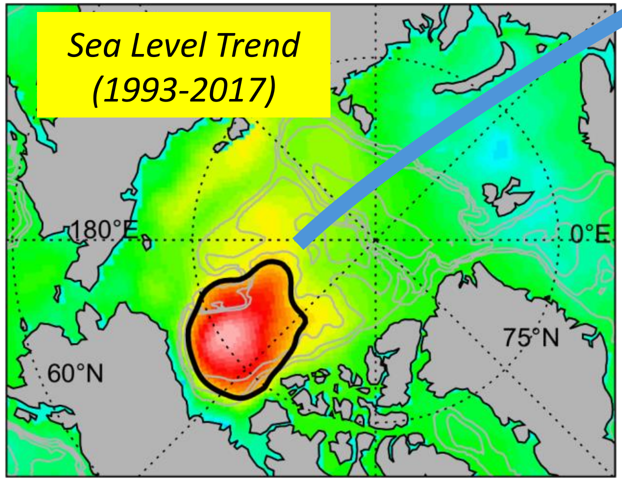
Control (forcing)

Sensitivity of J at a particular time T.

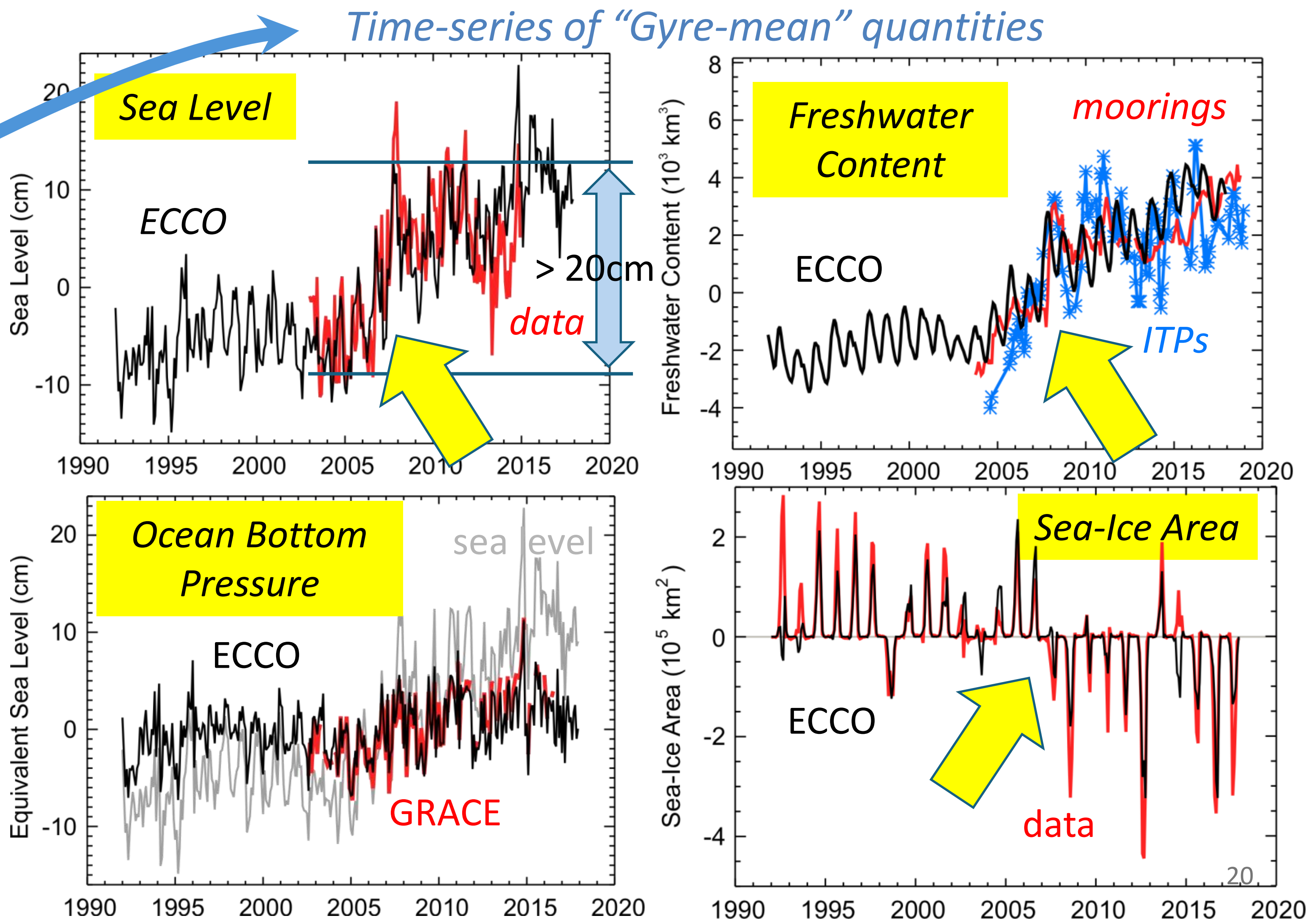
Sensitivity as a function of lag

Causation (2/9)

Sea level and freshwater content have been rising dramatically over the Beaufort Sea.

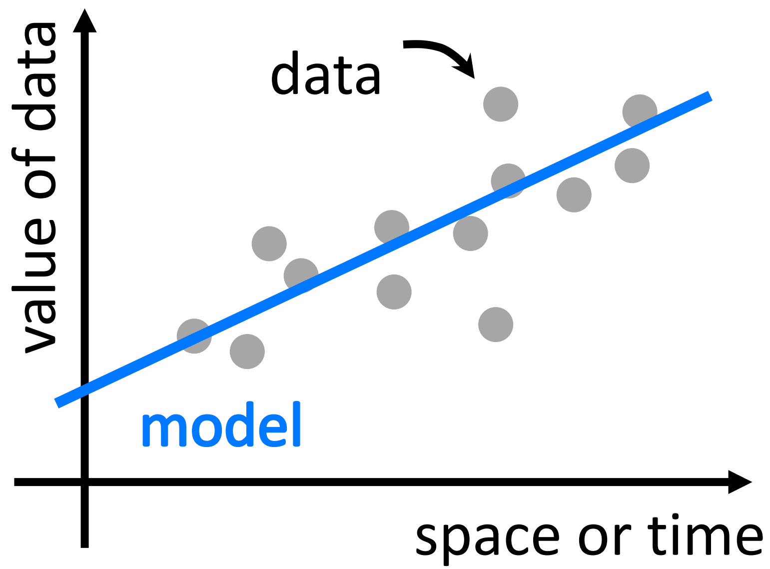


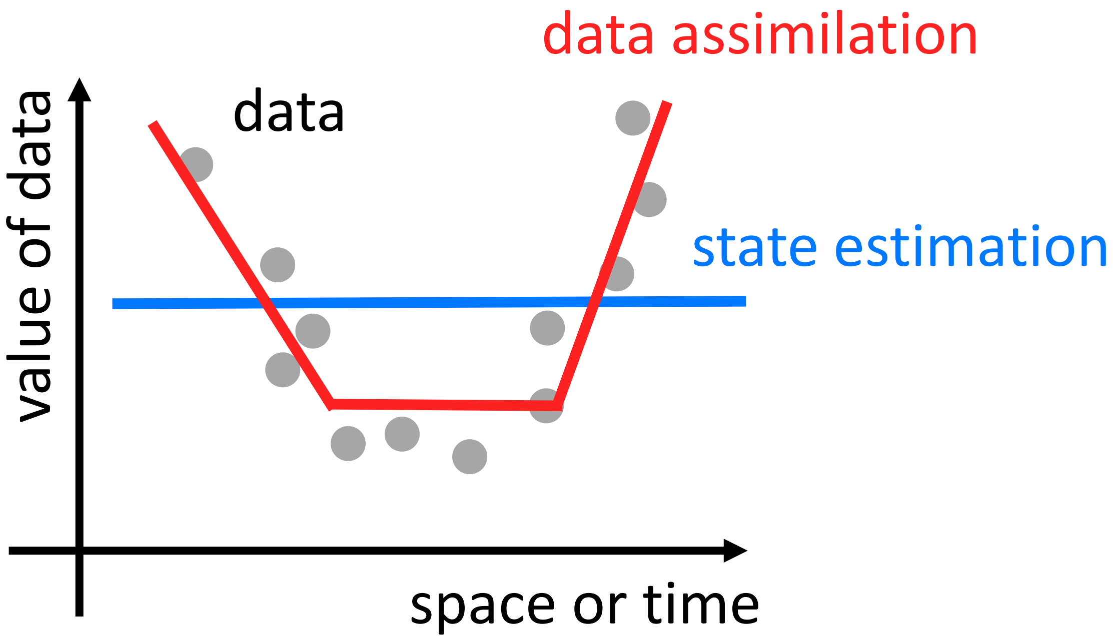
Fukumori, I., O. Wang, and I. Fenty (2021)
J. Phys. Oceanogr., **51**, 3217-3234,
https://doi.org/10.1175/JPO-D-21-0069.1.



Significance of Comparing with Data

Is comparison with observations meaningful if you are already constraining the model with that data?





Causation (3/9)

Adjoint Gradient Decomposition

Beaufort Sea mean sea level

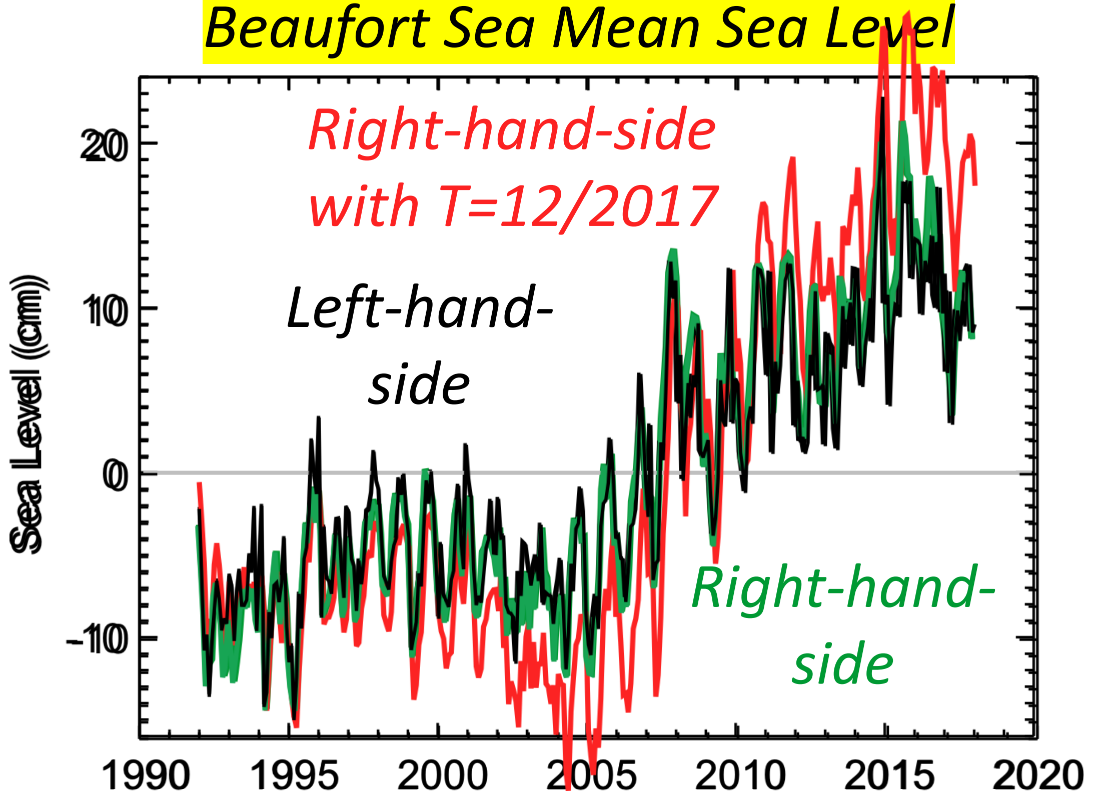
$$\delta J(t) \approx \sum_{i} \sum_{\mathbf{r}} \sum_{\Delta t} \frac{\partial J(T)}{\partial u_i(\mathbf{r}, T-\Delta t)} \delta u_i(\mathbf{r}, t-\Delta t)$$

Sensitivity (adjoint gradient) of J to forcing i

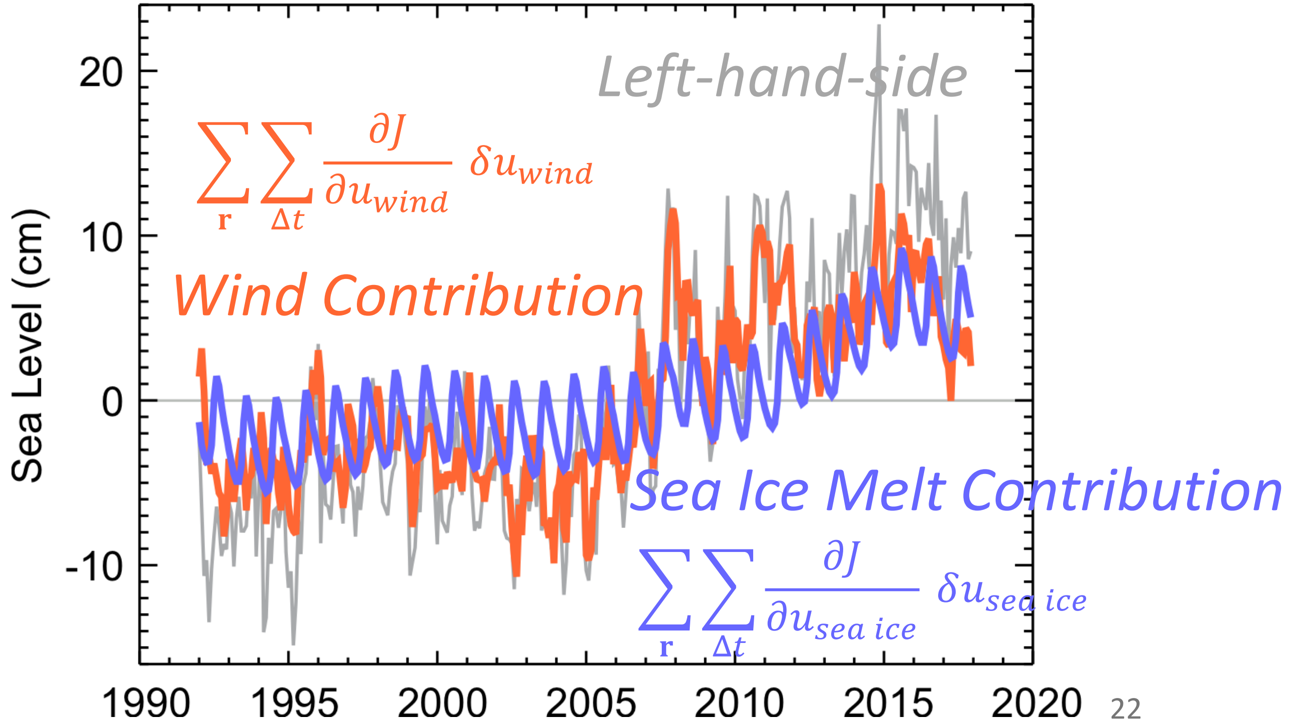
Forcing i

Forcings' Type Location Lag

Beaufort Sea Mean Sea Level



Decomposition (Type of Forcing)

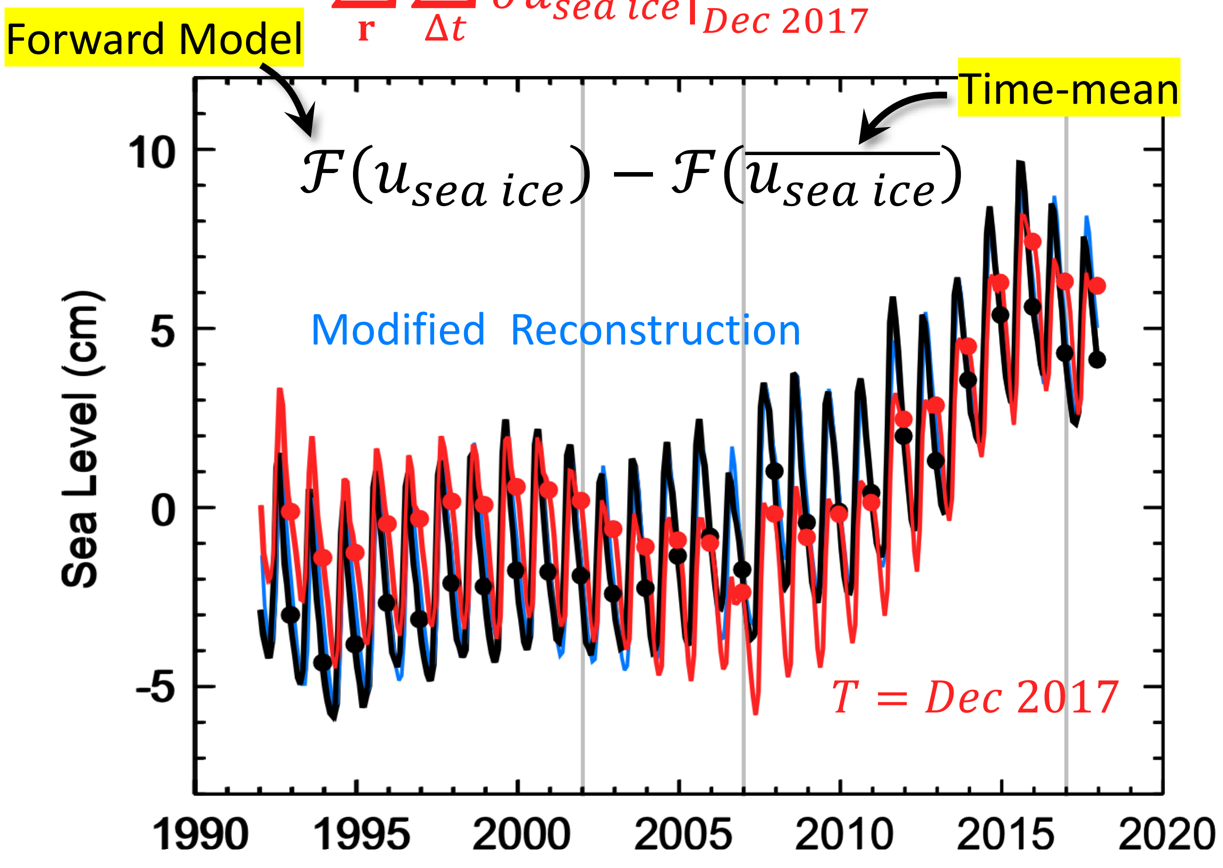


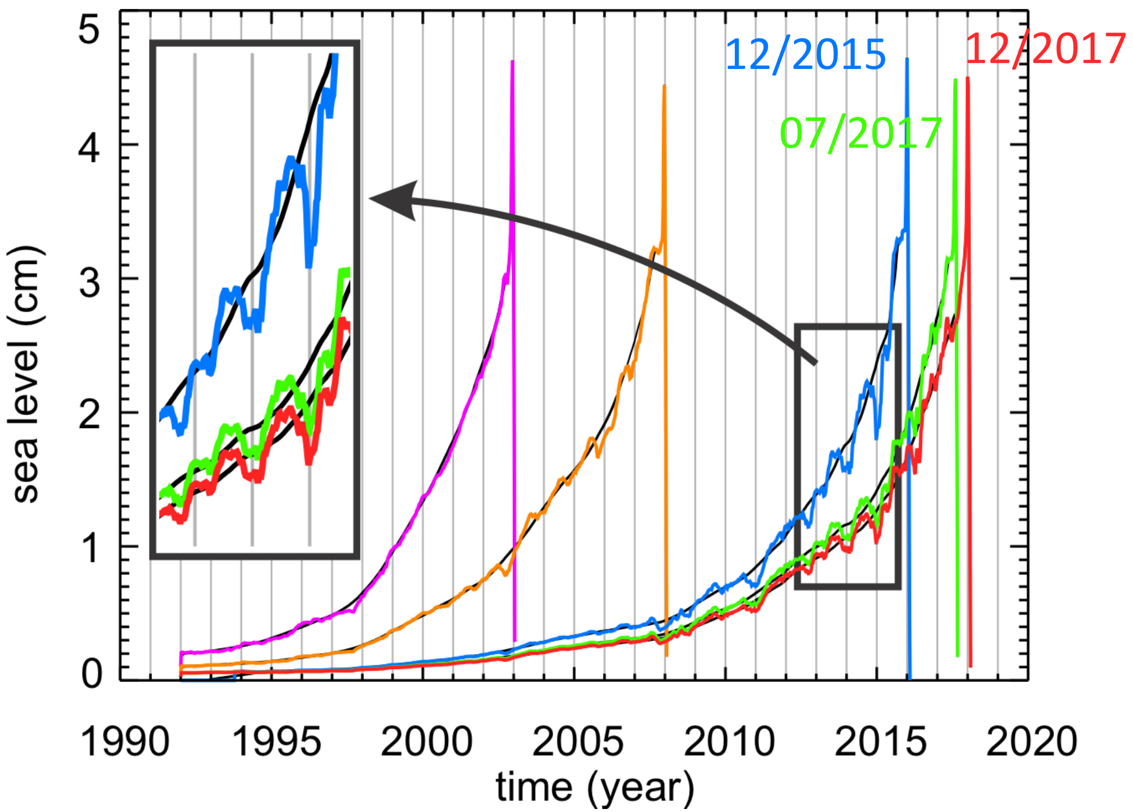
Causation (4/9)

Modified reconstruction of sea ice melt's contribution

$$\sum_{\mathbf{r}} \sum_{\Delta t} \left.\frac{\partial J}{\partial u_{sea\ ice}}\right|_{Dec\ 2017} \delta u_{sea\ ice}$$

$$\left.\frac{\partial J}{\partial u_{sea\ ice}}\right|_{T} \text{ near Gyre center}$$



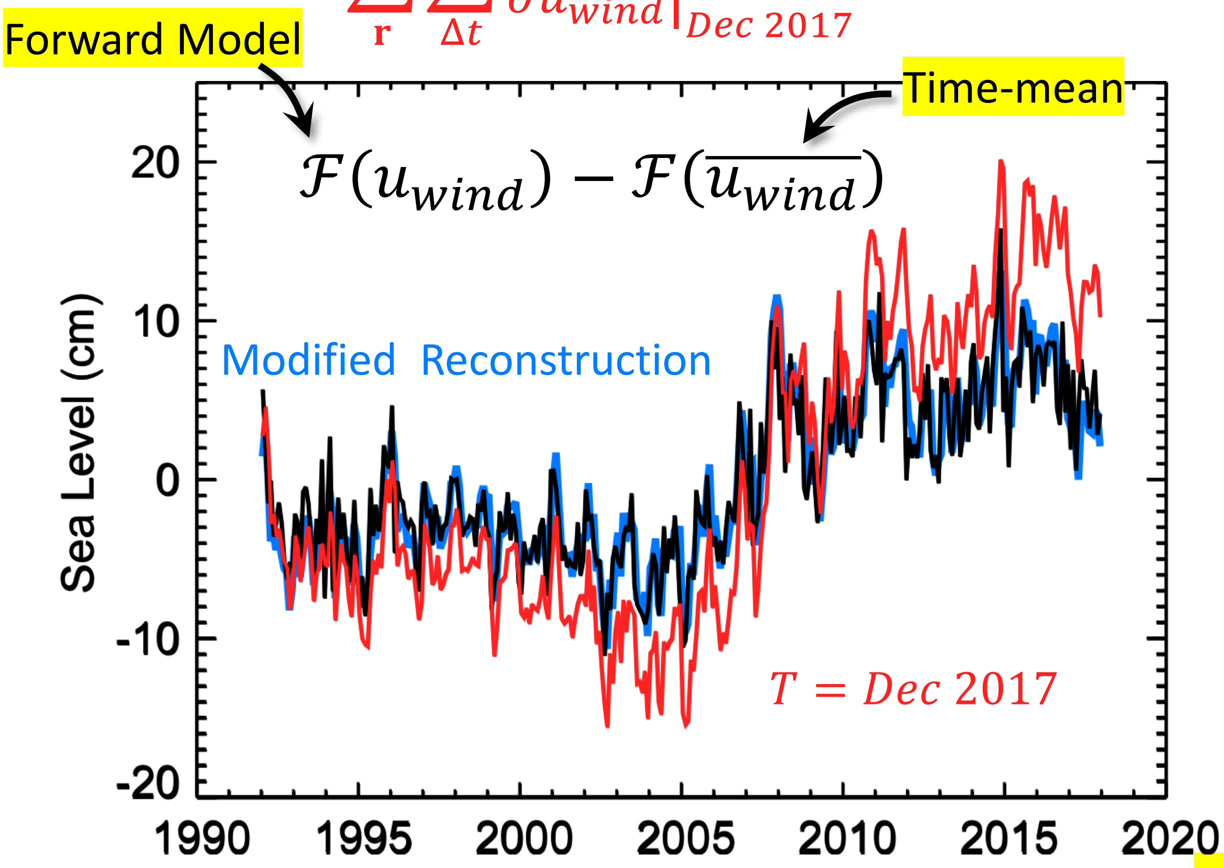


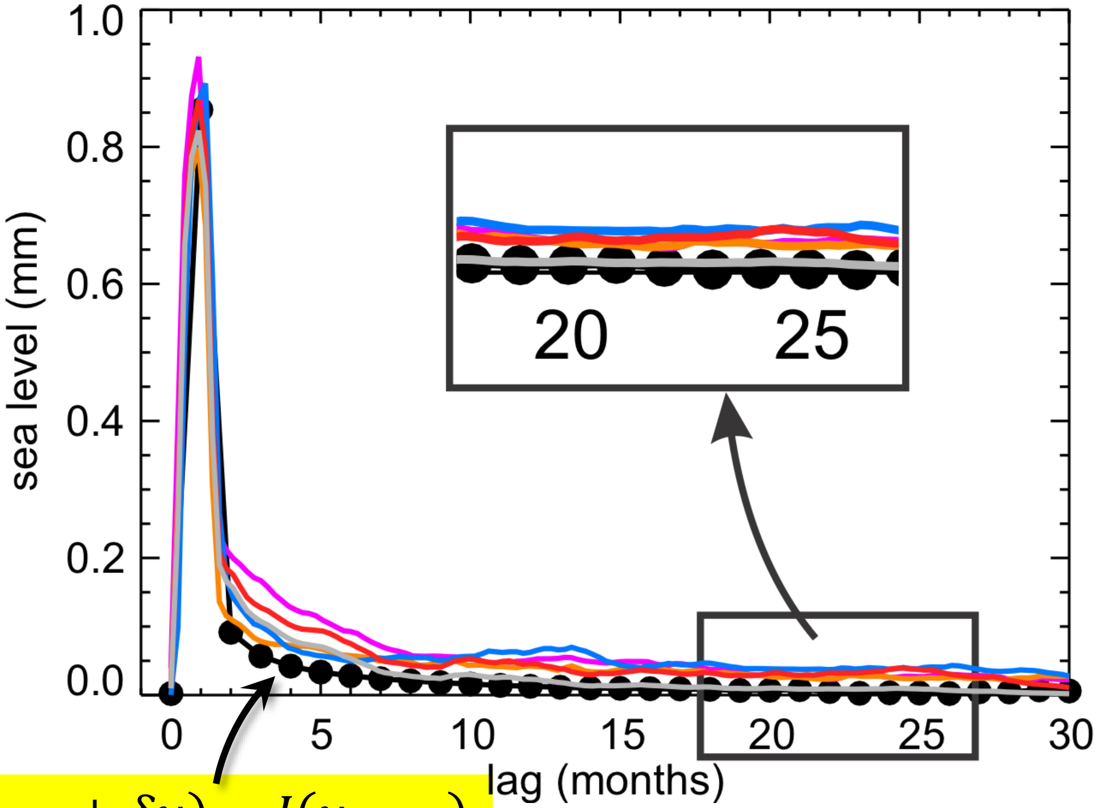
Causation (5/9)

Modified reconstruction of wind's contribution

$$\sum_{\mathbf{r}} \sum_{\Delta t} \frac{\partial J}{\partial u_{wind}}\bigg|_{Dec\ 2017} \quad \delta u_{wind}$$

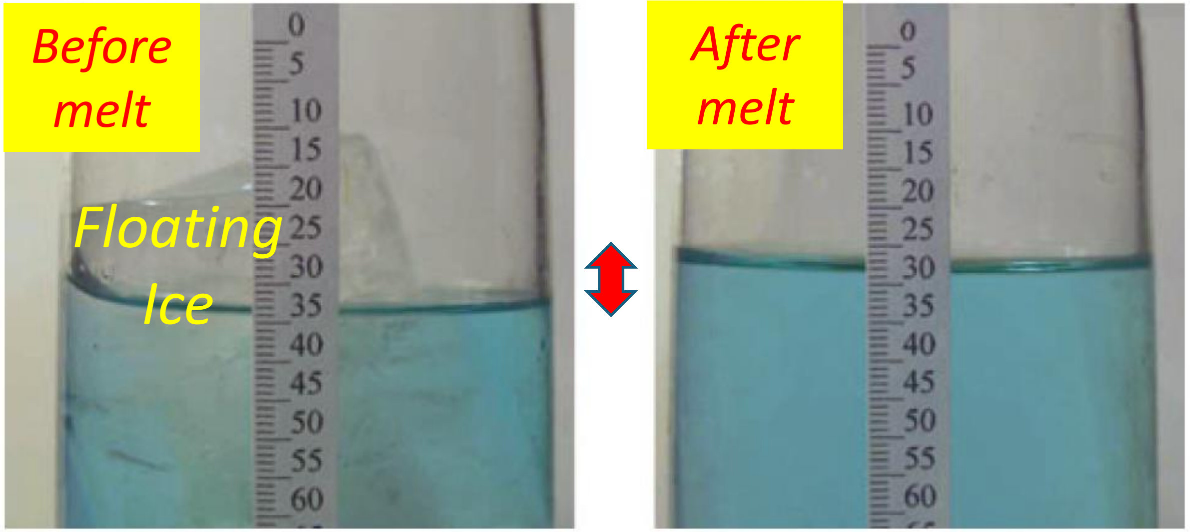
$$\frac{\partial J}{\partial u_{wind}}\bigg|_{T}$$ near southern edge of Gyre





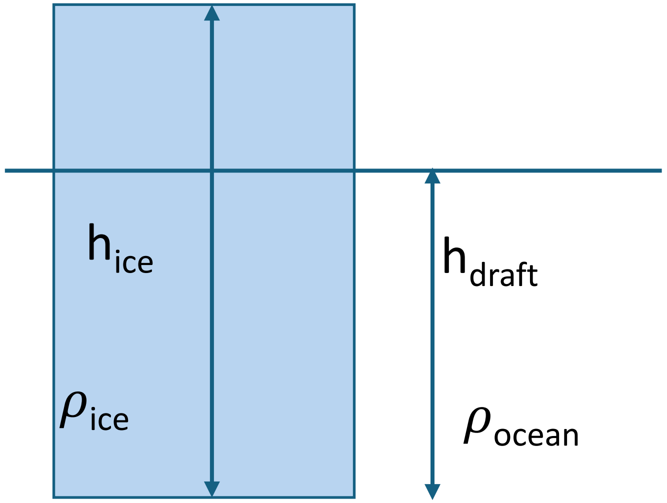
$$\frac{J(u_{wind} + \delta u) - J(u_{wind})}{\delta u}$$

Causation (6/9)



[Noerdlinger & Brower (2007)]

Sea level rises when floating sea ice melts, because melt water is fresher and occupies a larger volume than sea water displaced by ice.



Archimedes's Principle

Mass Conservation

$$\rho_{ocean} h_{draft} = \rho_{ice} h_{ice} = \rho_{fresh} h_{melt}$$

Therefore, $h_{melt} = \frac{\rho_{ocean}}{\rho_{fresh}} h_{draft} > h_{draft}$

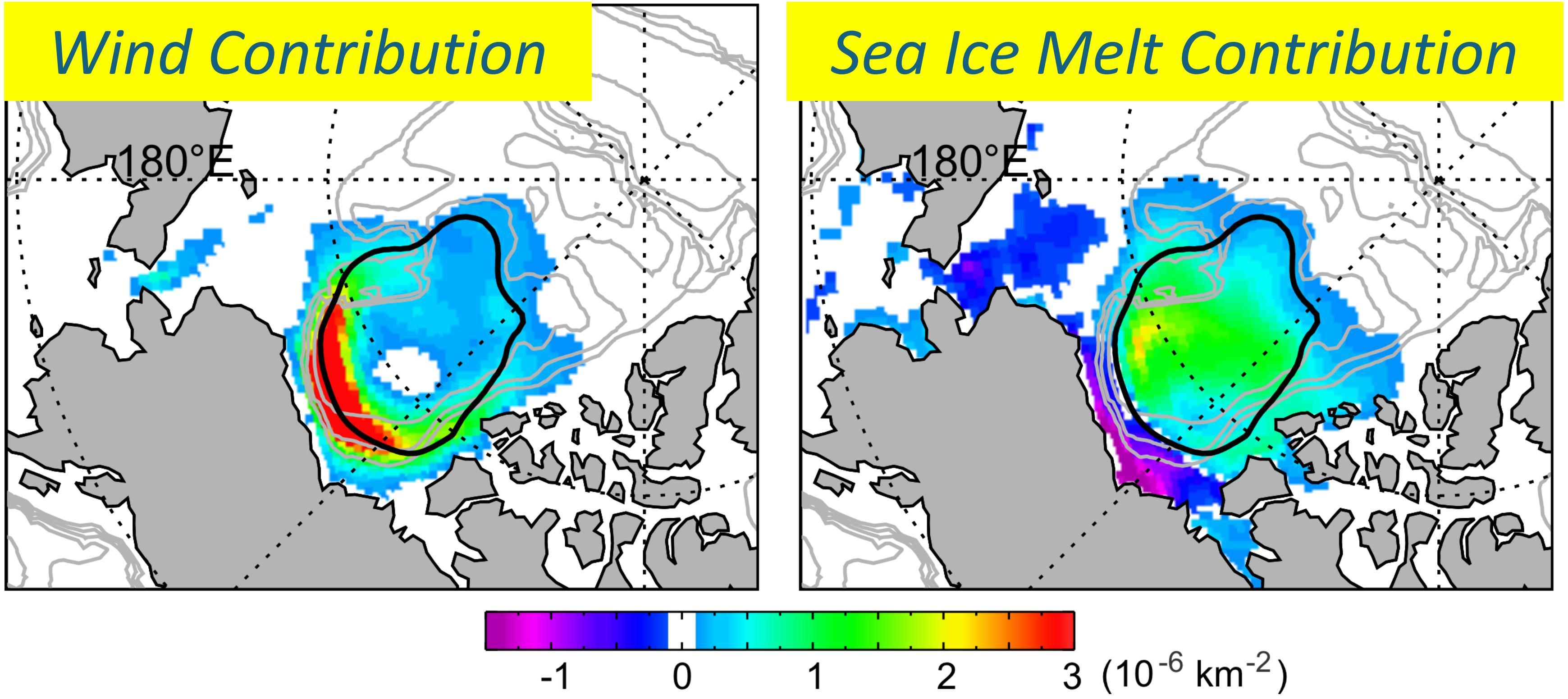
because $\frac{\rho_{ocean}}{\rho_{fresh}} \approx \frac{1026}{1000} \approx 2.6\%$ increase

Causation (7/9)

Wind-driven Ekman transport from the surrounding area and sea ice melt within the Gyre are responsible for the steric change.

Beaufort Sea's halosteric variance explained at different locations **r**.

$$E_i(\mathbf{r}) \equiv \frac{1}{dS(\mathbf{r})} \times \left[1 - \frac{\operatorname{var}\left\{ J_{halosteric}(t) - \sum_{\Delta t} \frac{\partial J(t_g)}{\partial \phi_i(\mathbf{r}, t_g - \Delta t)} \delta\phi_i(\mathbf{r}, t - \Delta t) \right\}}{\operatorname{var}\left\{ J_{halosteric}(t) \right\}} \right]$$

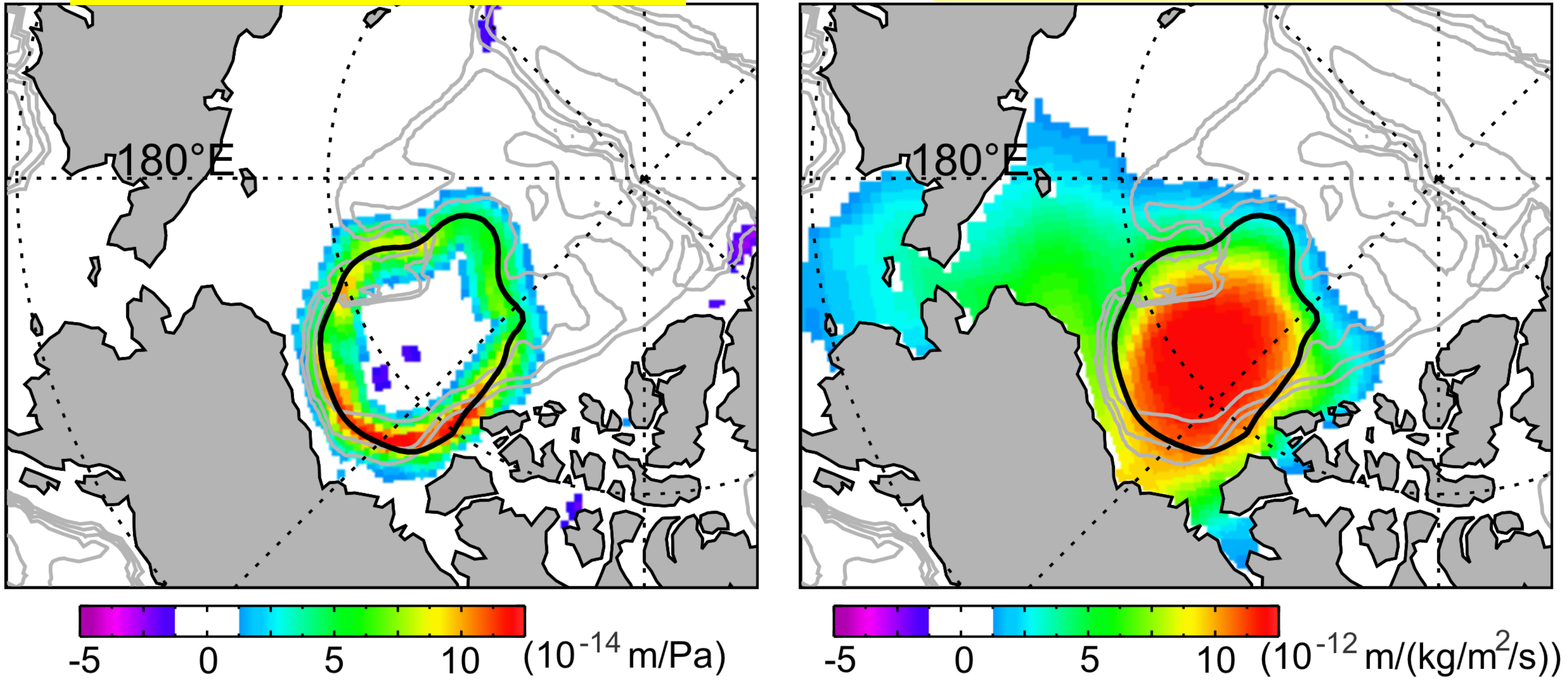


Causation (8/9)

The *gradients* illustrate the role of wind-driven Ekman flux and the ocean’s circulation pathway.

Clockwise along-boundary surface stress at 8-weeks lag

Surface freshwater flux at 78-weeks lag

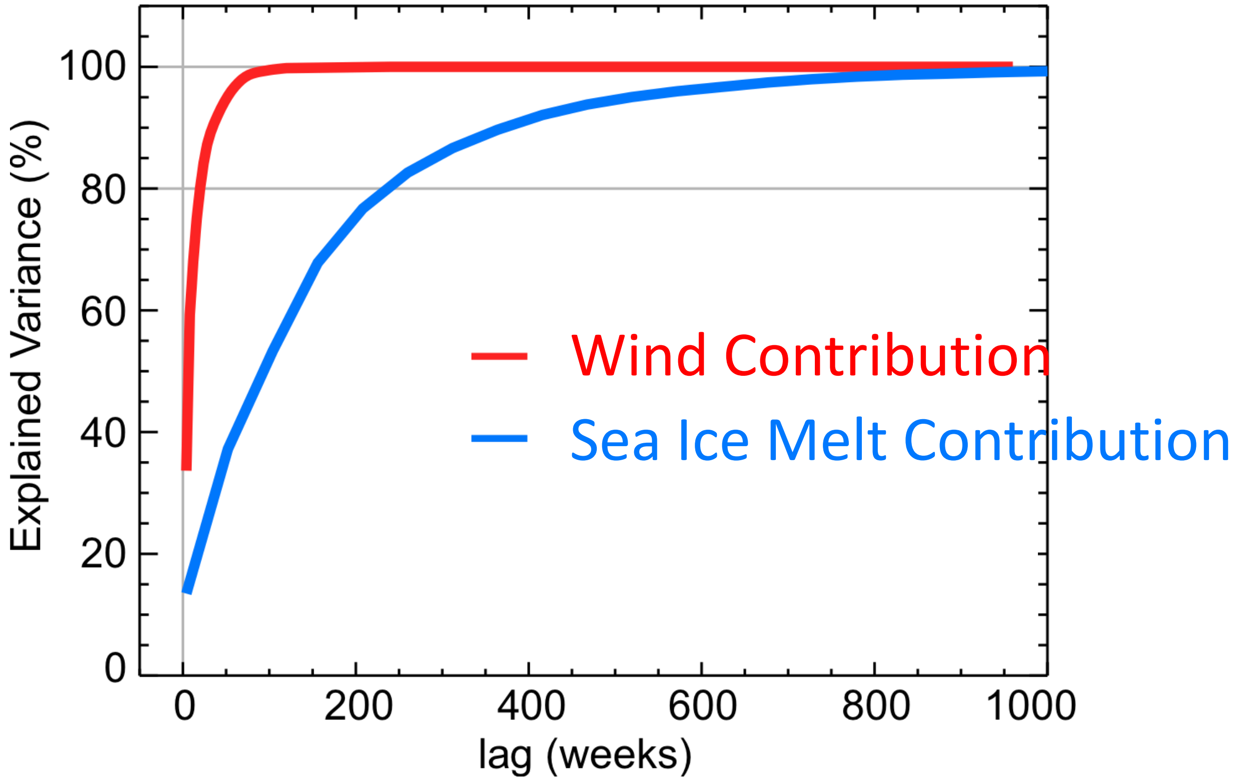


Causation (9/9)

Effects of wind last only a <u>few months</u>, but
effects of sea ice melt last for <u>years</u>.

Explained variance
vs maximum lag
(cumulative skill)

$$E_i\left(0 \le \Delta t \le T\right) = 1 - \frac{\operatorname{var}\left\{\delta J_i(t) - \sum_{\mathbf{r}} \sum_{\Delta t=0}^{T} \frac{\partial J(t_g)}{\partial \phi_i(\mathbf{r}, t_g - \Delta t)} \delta\phi_i(\mathbf{r}, t-\Delta t)\right\}}{\operatorname{var}\left\{\delta J_i(t)\right\}}$$



Example Studies Using Adjoint Gradient Decomposition

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Summary

- Adjoint is a transformation for studying mathematical relationships,
- Adjoint models compute gradients efficiently for specific objective functions (numerator),
- Adjoints enable functional analysis of models, i.e., “*model calculus*”,
  - Circulation pathways (adjoint passive tracers),
  - Causal relationships (Adjoint Gradient Decomposition).

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