More than gradients:

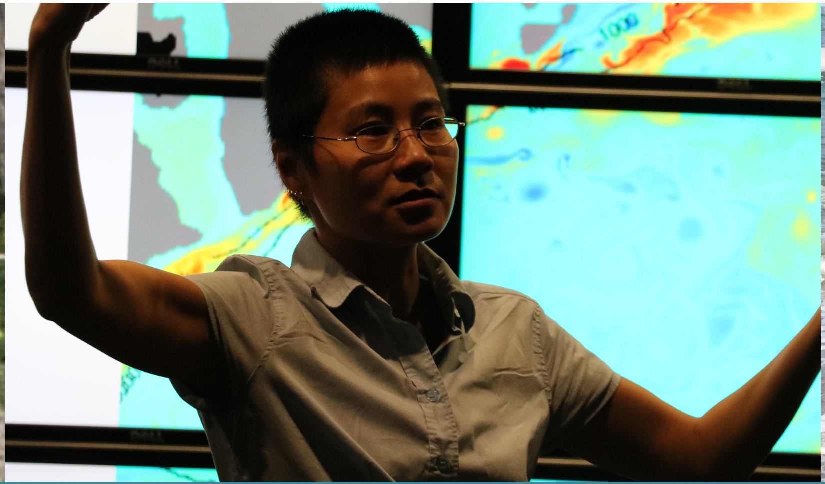
Dynamical attribution in ocean science using adjoint models

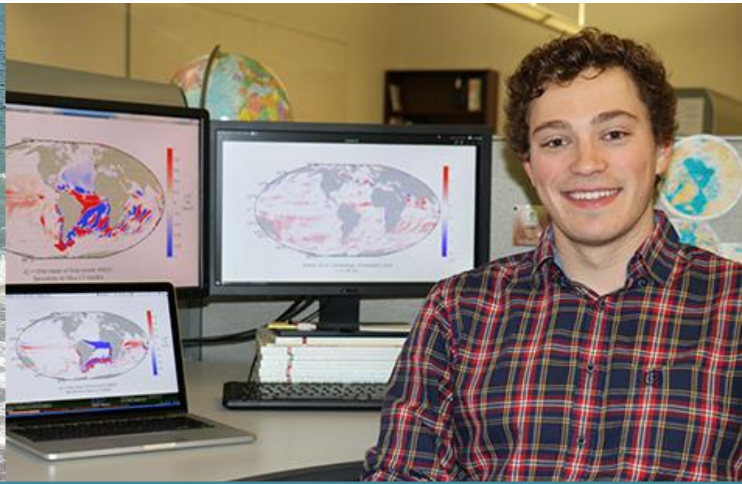
Patrick Heimbach (messenger), Nora Loose, An T. Nguyen, Helen Pillar, Timothy Smith, and others …

Oden Institute for Computational Engineering and Sciences

Institute for Geophysics, Jackson School of Geosciences

The University of Texas at Austin





Overview

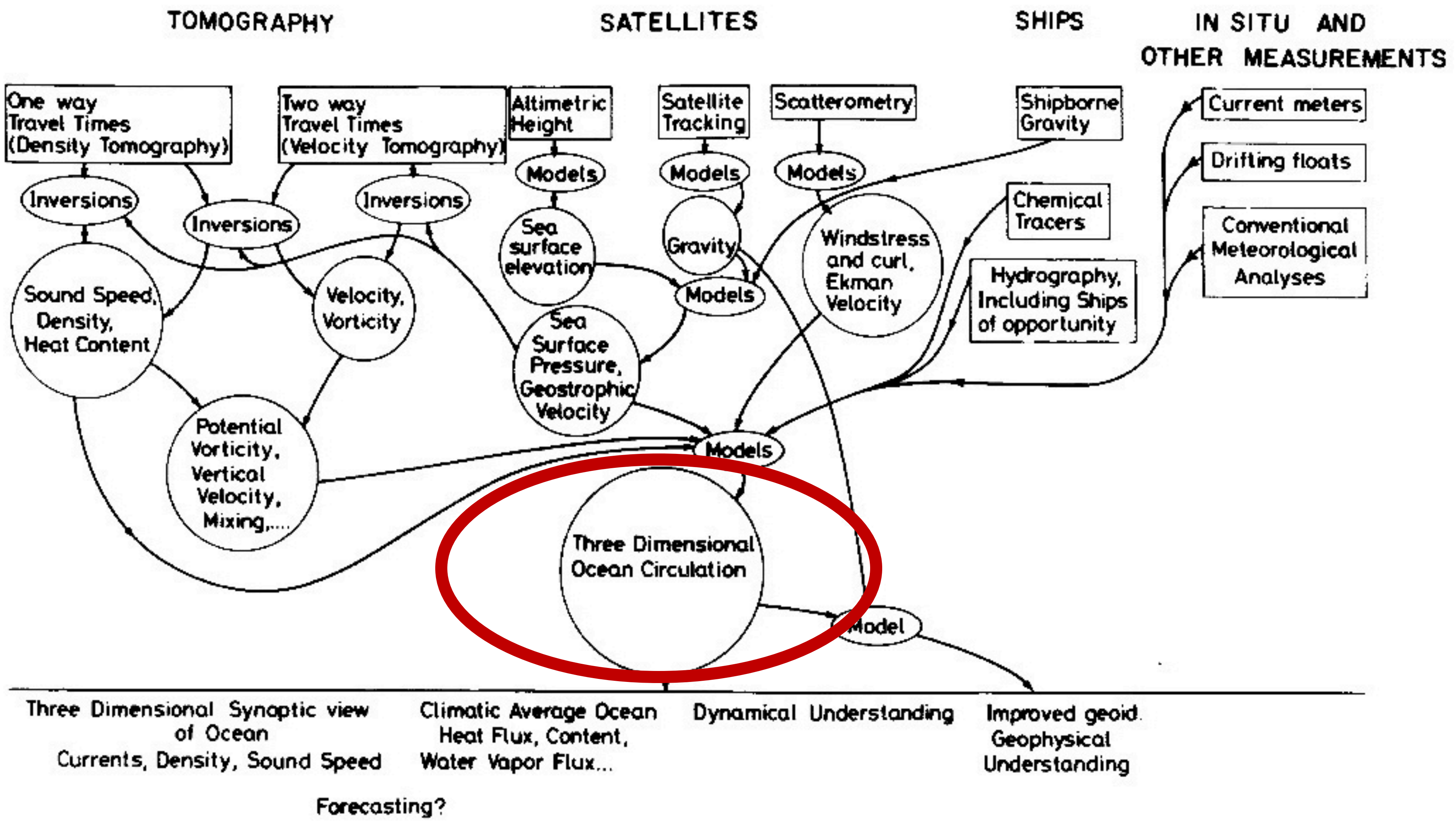
1. Short recap: the global ocean circulation inverse *problem*
2. The adjoint (or Lagrange multiplier) method
   - Getting the adjoint of a GCM
3. Causal / dynamical attribution based on the *dual* ocean state
   - Application to the North Atlantic circulation

1.

Short recap:
The ocean circulation inverse problem

The ocean circulation inverse problem – historical

Drawn by Carl Wunsch on the occasion of Walter Munk's 65th Birthday, 1982



Munk & Wunsch: Observing the Ocean in the 1990s. *Phil. Trans. R. Soc. Lon. A* (1982)

The ocean circulation inverse problem – today

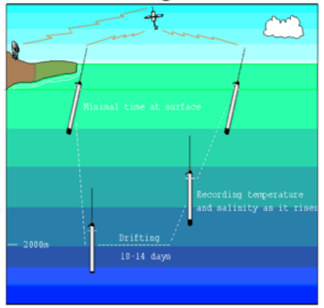
Estimating the Circulation and Climate of the Ocean (ECCO)

Stammer et al., JGR (2002)

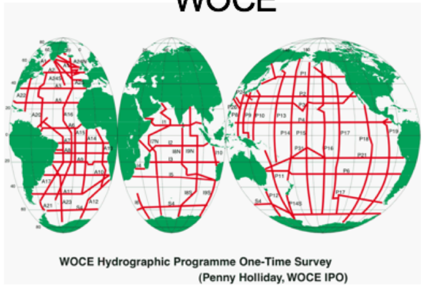
Wunsch & Heimbach, Physica D (2007)

http://ecco-group.org

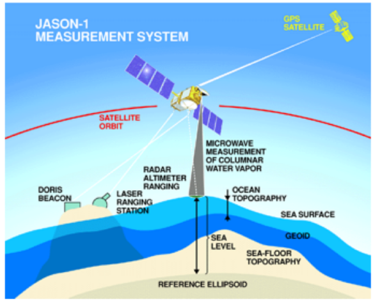
Argo



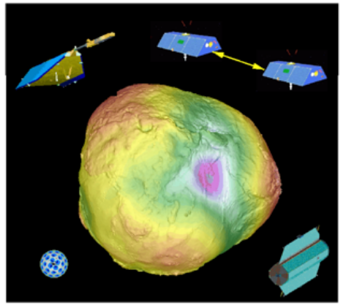
WOCE



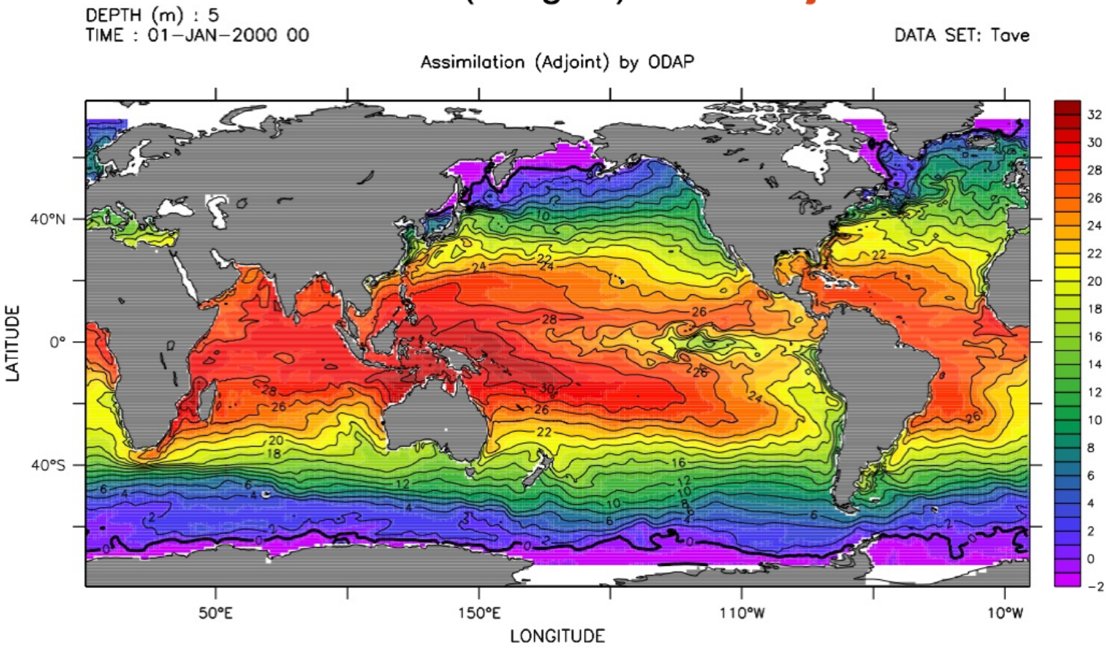
T/P, Jason



GRACE



How to synthesize? Estimation/optimal control problem:
Use a **model** (MITgcm) and its **adjoint**:



INSTITUTE FOR COMPUTATIONAL ENGINEERING & SCIENCES

The ocean circulation inverse problem

Consider model L, and observation y with noise ϵ:

$$x_{k+1} = L\, x_k\,, \quad \text{and} \quad y_{k+1} = E\, x_{k+1} + \epsilon_{k+1}$$

Variational form of least-squares estimation problem:

$$\mathcal{J}(x) = \sum_{0 \le k \le N} \left[E\, x_k - y_k\right]^T \mathbf{R}^{-1} \left[E\, x_k - y_k\right] + \left[x_k - x^b\right]^T \mathbf{B}^{-1} \left[x_k - x^b\right], \quad t = k\Delta t$$

Extend to Lagrange function $\mathcal{L}$, Lagrange multipliers μ_k:

$$\mathcal{L}(x, \mu) = J(x) + \sum_{0 \le k \le N} \mu_k^T \left[x_{k+1} - L\, x_k\right]$$

Wunsch & Heimbach
Physica D (2007)

The ocean circulation inverse problem

Lagrange multiplier method:

Stationary point of $\mathcal{L}$ leads to set of normal equations:

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}(t)} &= \mathbf{x}(t) - L\left[\mathbf{x}(t-1)\right] = 0 && 1 \leq t \leq t_f \\
\frac{\partial \mathcal{L}}{\partial \mathbf{x}(t)} &= \frac{\partial J_0}{\partial \mathbf{x}(t)} - \boldsymbol{\mu}(t) && \\
&\quad + \left[\frac{\partial L[\mathbf{x}(t)]}{\partial \mathbf{x}(t)}\right]^T \boldsymbol{\mu}(t+1) = 0 && 0 < t < t_f \\
\frac{\partial \mathcal{L}}{\partial \mathbf{x}(t_f)} &= \frac{\partial J}{\partial \mathbf{x}(t_f)} - \boldsymbol{\mu}(t_f) = 0 && t = t_f \\
\frac{\partial \mathcal{L}}{\partial \mathbf{x}(0)} &= \frac{\partial J}{\partial \mathbf{x}(0)} - \left[\frac{\partial L[\mathbf{x}(0)]}{\partial \mathbf{x}(0)}\right]^T \boldsymbol{\mu}(1) && t_0 = 0
\end{aligned}
$$

Wunsch & Heimbach
Physica D (2007)

The ocean circulation inverse problem

$$\mu_0 = \frac{\partial J}{\partial x_0} = \sum_{1 \le k \le N} \frac{\partial x_k}{\partial x_0} \left(\frac{\partial J}{\partial x_k} \right)$$

$$= \frac{\partial x_1}{\partial x_0} \left(\frac{\partial J}{\partial x_1} \right) + \frac{\partial x_1}{\partial x_0} \frac{\partial x_2}{\partial x_1} \left(\frac{\partial J}{\partial x_2} \right) + \ldots + \frac{\partial x_1}{\partial x_0} \cdots \frac{\partial x_N}{\partial x_{N-1}} \left(\frac{\partial J}{\partial x_N} \right)$$

$$= \mathbf{L}^T \frac{\partial J}{\partial x_1} + \mathbf{L}^T \mathbf{L}^T \frac{\partial J}{\partial x_2} + \ldots + \mathbf{L}^T \cdots \mathbf{L}^T \frac{\partial J}{\partial x_N}$$

$\mathbf{L}^T$: is the **adjoint model** (and $\mathbf{L}$ is the **tangent linear model**)

$\mu_k = \left(\frac{\partial J}{\partial x_k} \right)$: **Lagrange multipliers** or **gradients**

Wunsch & Heimbach Physica D (2007)

2.
Getting the adjoint of an ocean general circulation model

Some of the challenges:

Generating & maintaining the adjoint of a state-of-the-art ocean circulation model

$$\frac{D\vec{\mathbf{v}}_h}{Dt} + f\hat{\mathbf{k}} \times \vec{\mathbf{v}}_h + \frac{1}{\rho_c}\nabla_z p = \vec{\mathcal{F}}$$

$$\epsilon_{nh}\frac{Dw}{Dt} + \frac{g\rho}{\rho_c} + \frac{1}{\rho_c}\frac{\partial p}{\partial z} = \epsilon_{nh}\mathcal{F}_w$$

$$\nabla_z \cdot \vec{\mathbf{v}}_h + \frac{\partial w}{\partial z} = 0$$

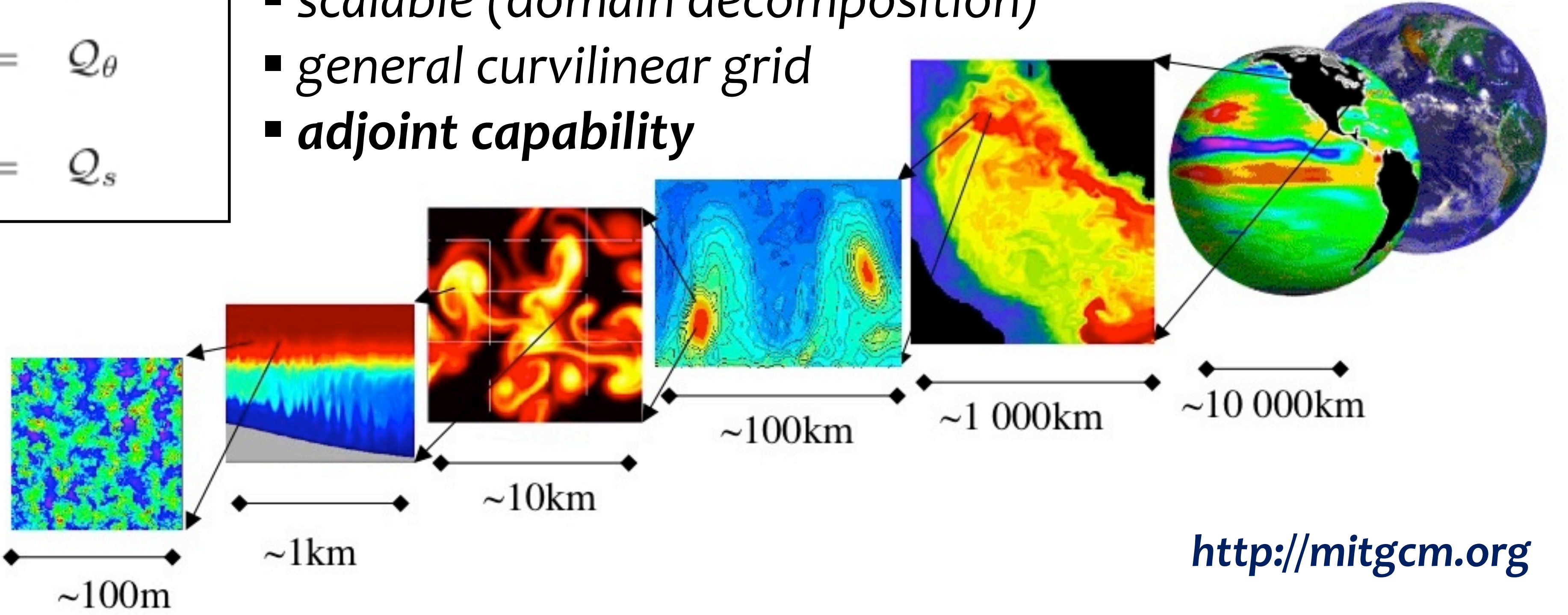
$$\rho = \rho(\theta, S)$$

$$\frac{D\theta}{Dt} = \mathcal{Q}_\theta$$

$$\frac{DS}{Dt} = \mathcal{Q}_s$$

Approx. form of Navier-Stokes equations for incompressible fluid:

- *momentum equation (including Coriolis term)*
- *conservation of mass – NLFS & real water flux*
- *conservation of tracers (heat, salt)*
- *nonlinear equation of state for sea water*
- *subgrid-scale parameterizations*
- *scalable (domain decomposition)*
- *general curvilinear grid*
- ***adjoint capability***

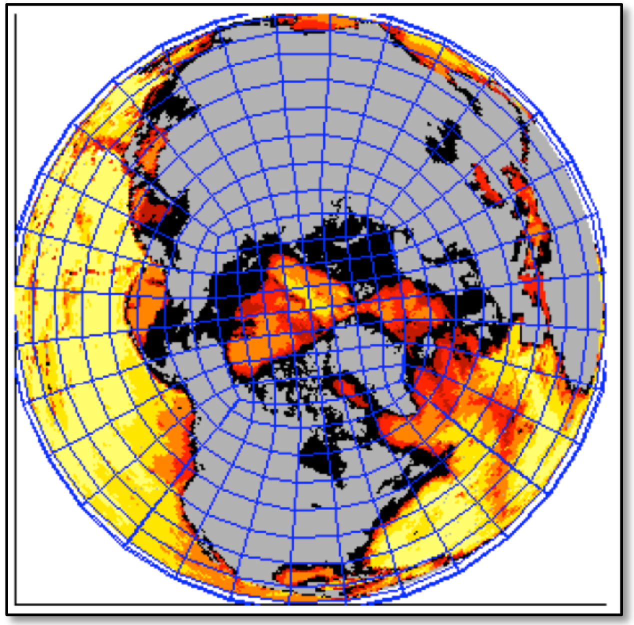


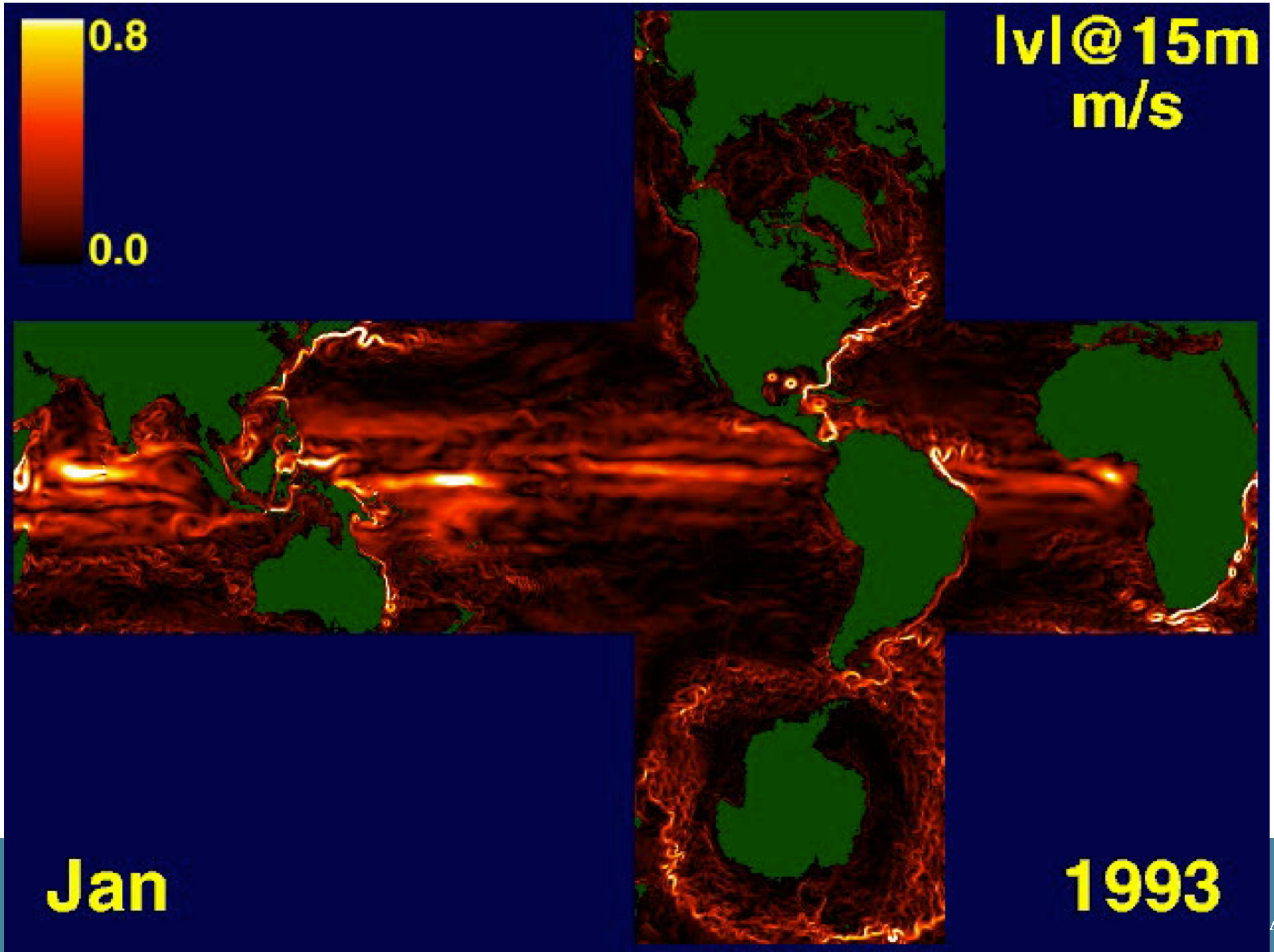
http://mitgcm.org

Some of the challenges:

Generating & maintaining the adjoint of a state-of-the-art ocean circulation model

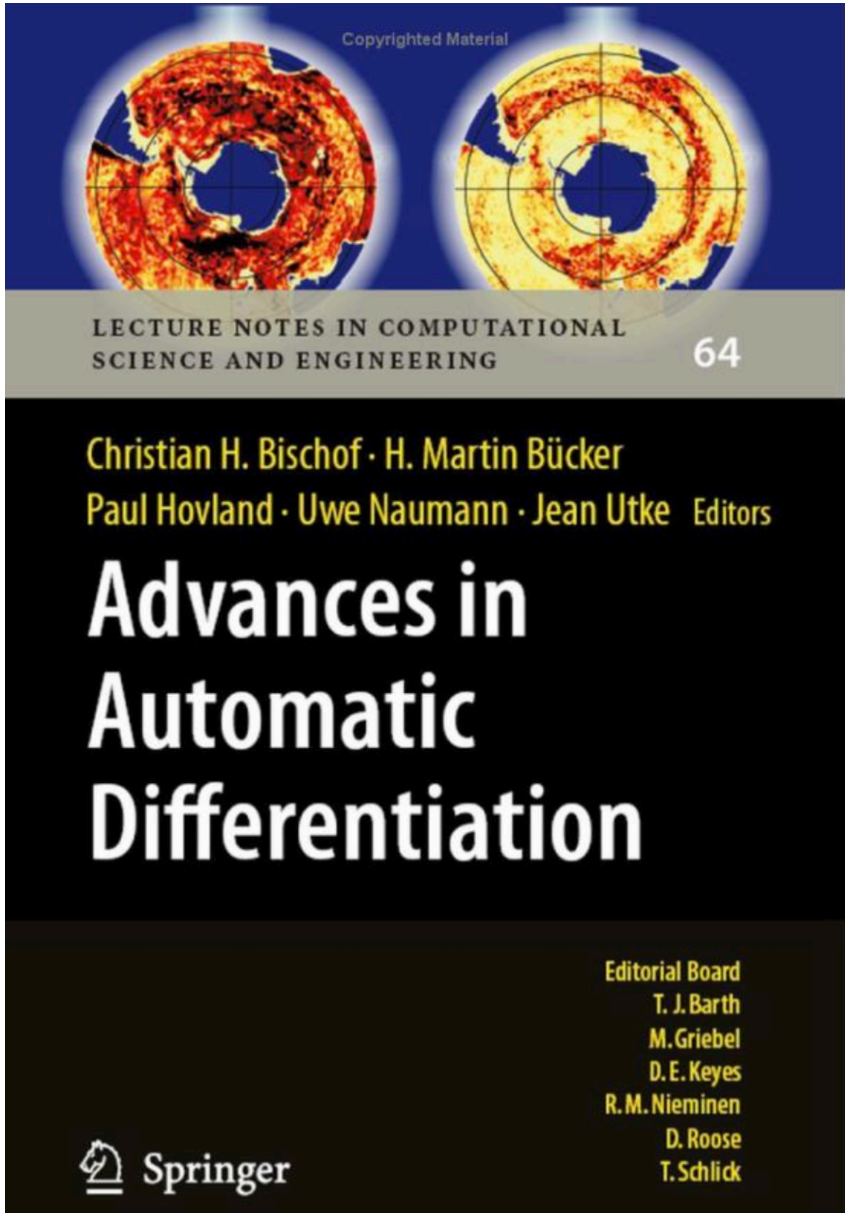
Global ocean simulation on a "cubed-sphere" grid topology



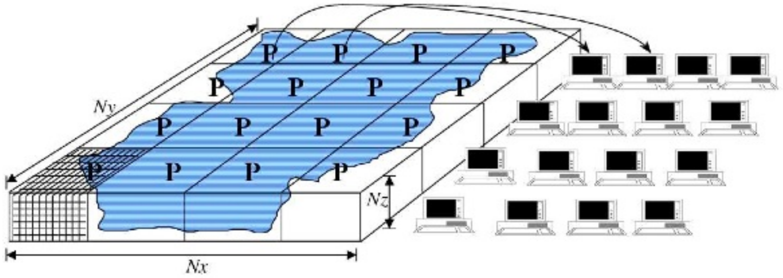


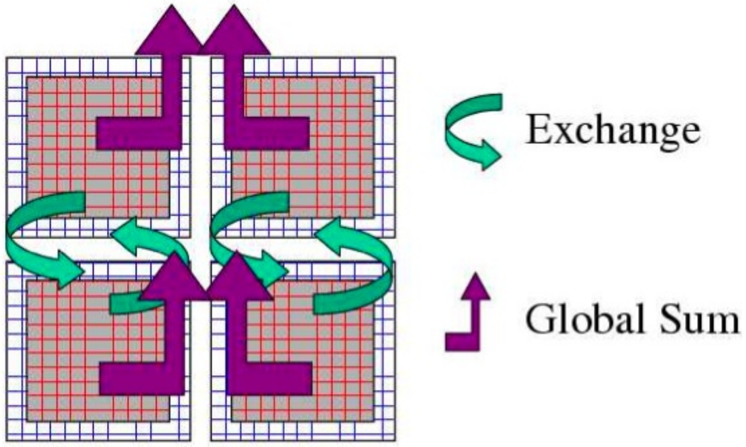
Some of the challenges:

Generating & maintaining the adjoint of a state-of-the-art ocean circulation model



- domain decomposition (tiles) & overlaps (halos)
- split into extensive on-processor and global phase

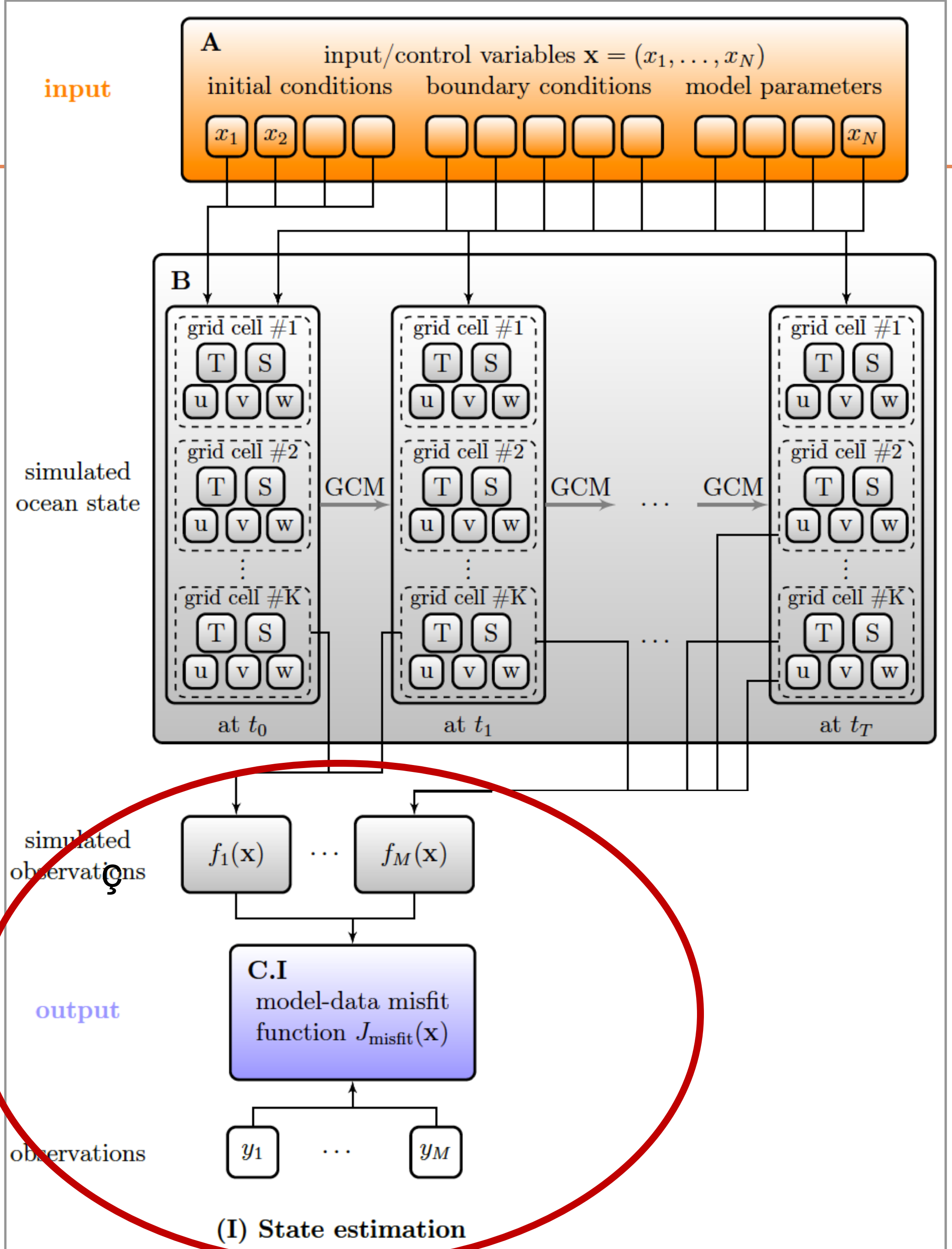




Global communication/arithmetic op.'s supported by MITgcm's intermediate layer (WRAPPER) which need hand-written adjoint forms

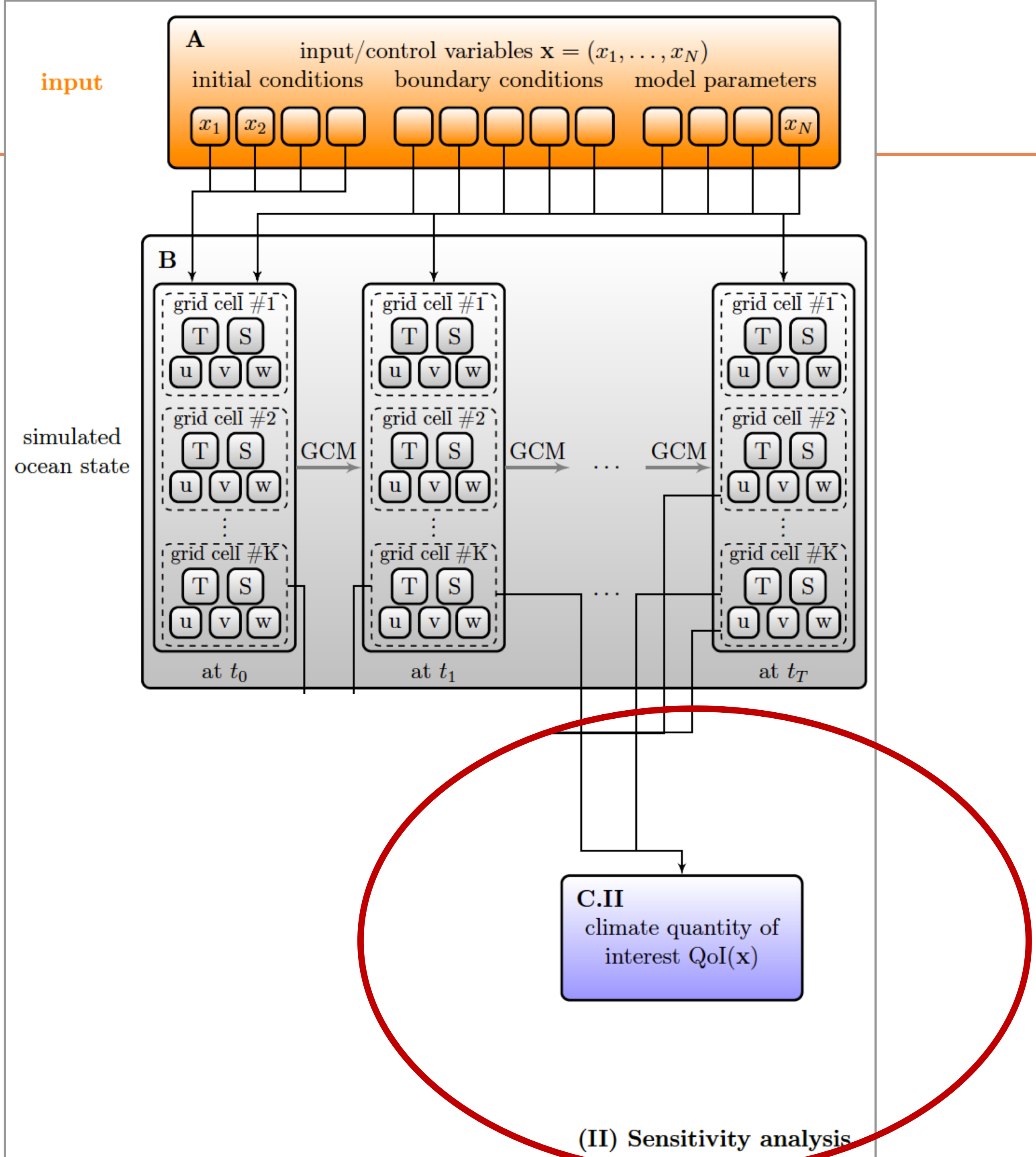
	operation/primitive	forward		reverse
•	communication (MPI,...):	send	$\longleftrightarrow$	receive
•	arithmetic (global sum,...):	gather	$\longleftrightarrow$	scatter
•	active parallel I/O:	read	$\longleftrightarrow$	write

The inverse problem



Courtesy Nora Loose

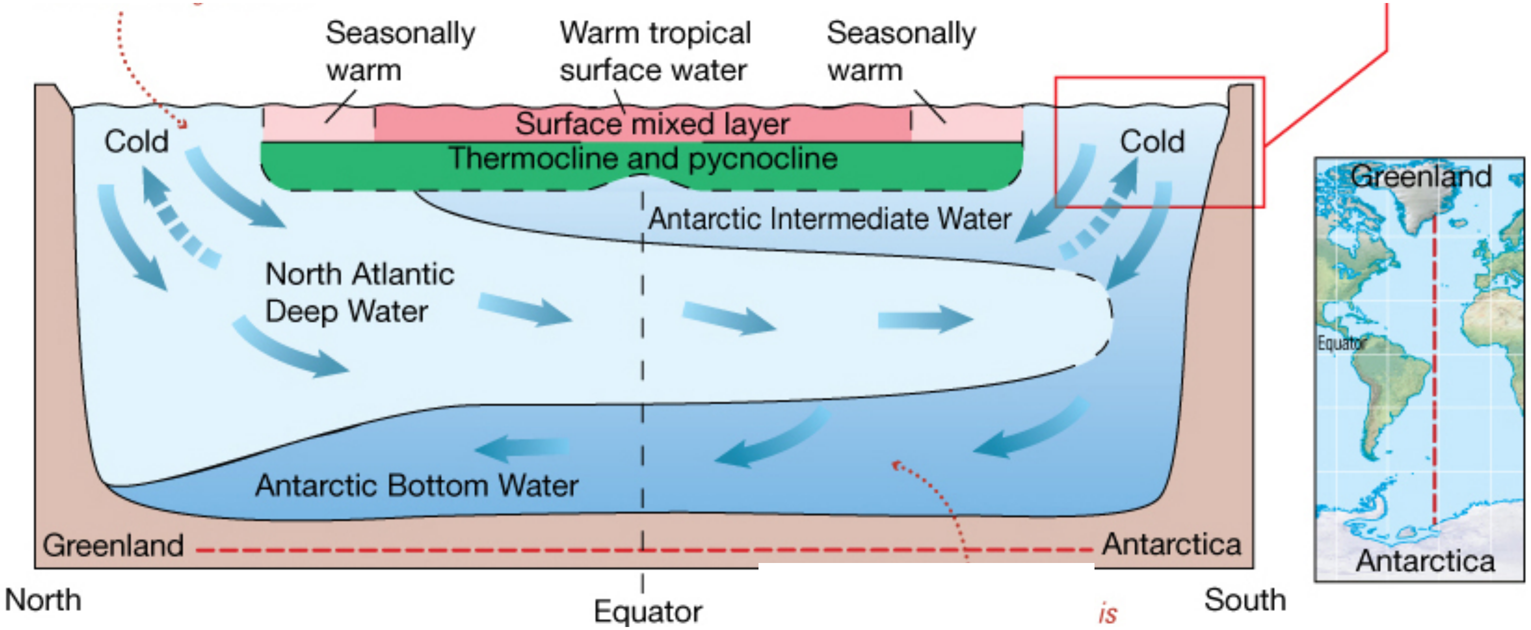
The sensitivity analysis problem

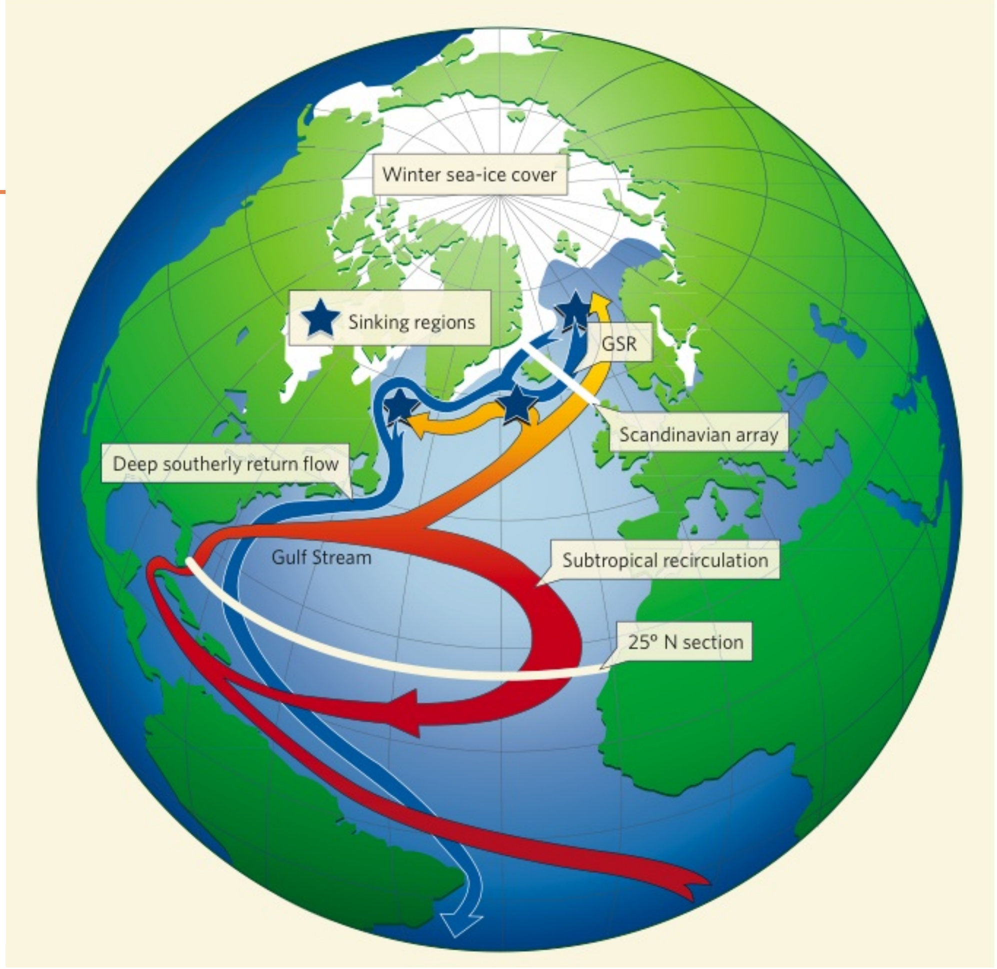


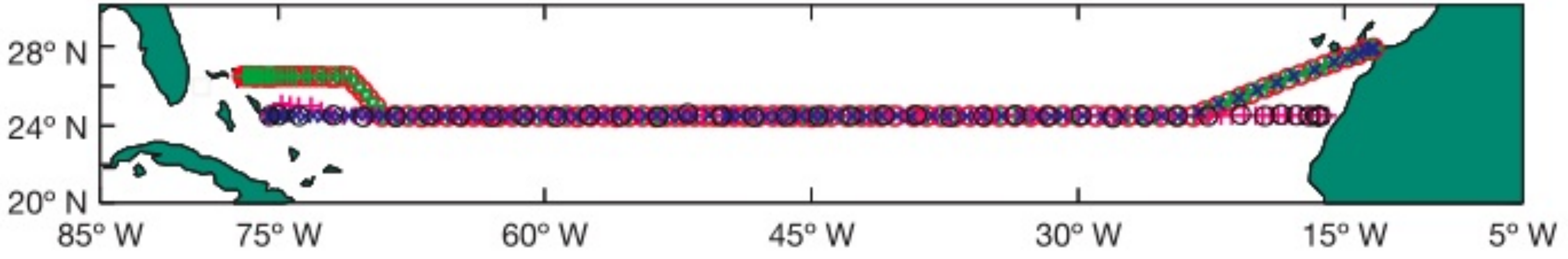
Courtesy Nora Loose

3.
Dynamical attribution
via the dual (adjoint) state

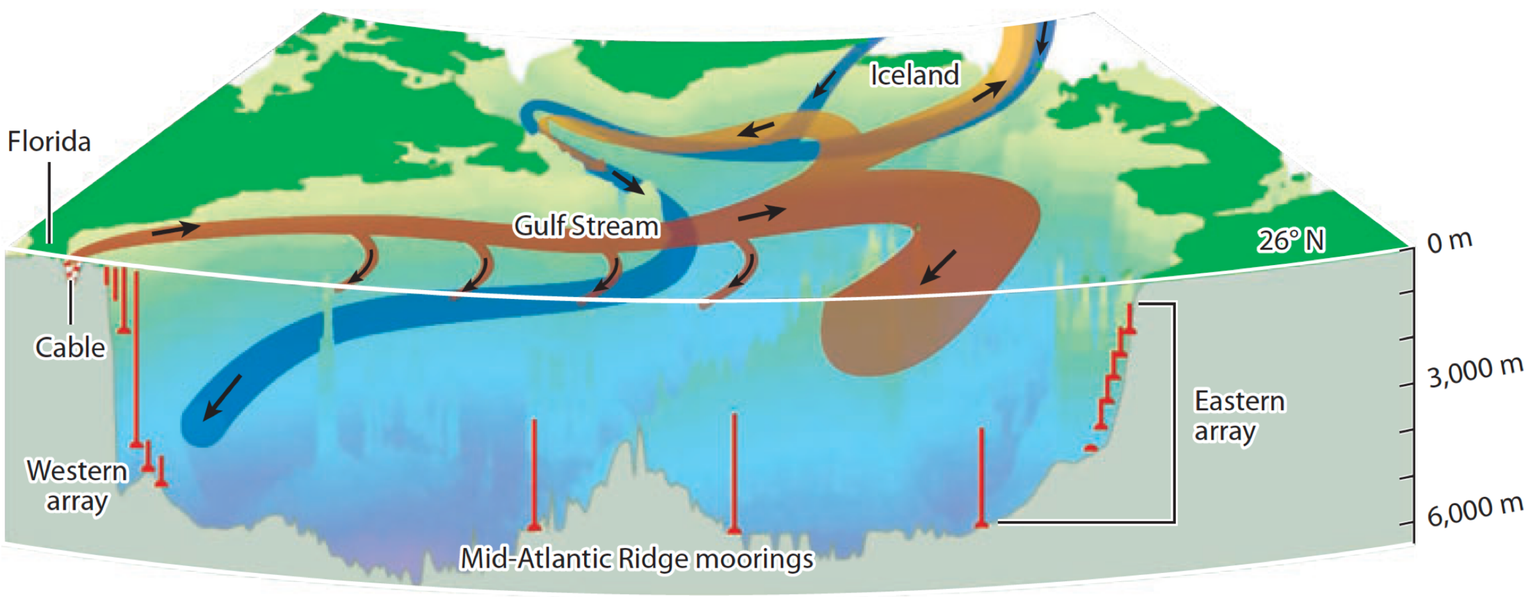
Dynamical attribution:
The Atlantic Meridional Overturning Circulation







Dynamical attribution:
The Atlantic MOC @ 26ºN



(North) Atlantic Meridional Overturning Circulation **(AMOC)** variability

Quantity of interest:

$$\delta \mathcal{J}(u(x,y,t)) \equiv \text{Monthly AMOC Anomaly}$$

"controlled" by:

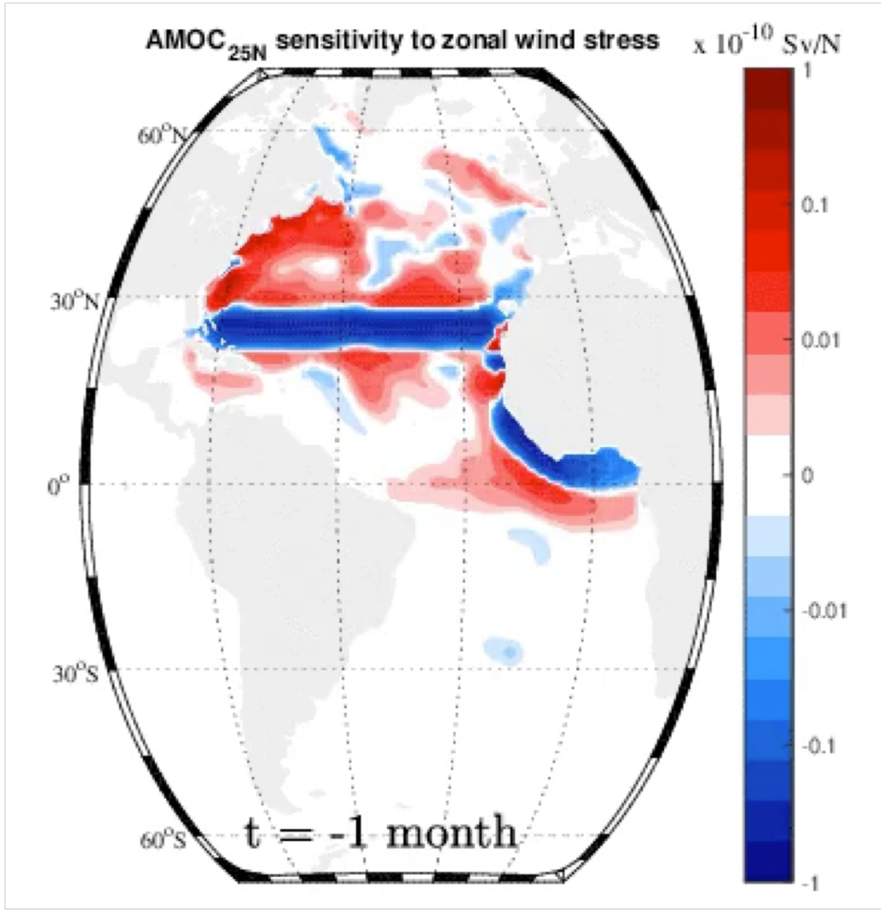
$$\delta u(x,y,t) \equiv \text{Surface Atm. Forcing Perturbations}$$

through (assumed) linear dynamics described by:

$$\frac{\partial \mathcal{J}}{\partial u}(x,y,t) \equiv \text{Sensitivity}$$

Dynamical attribution:

The Atlantic MOC @ 26°N



Pillar et al., J. Clim. (2016)

Recall:

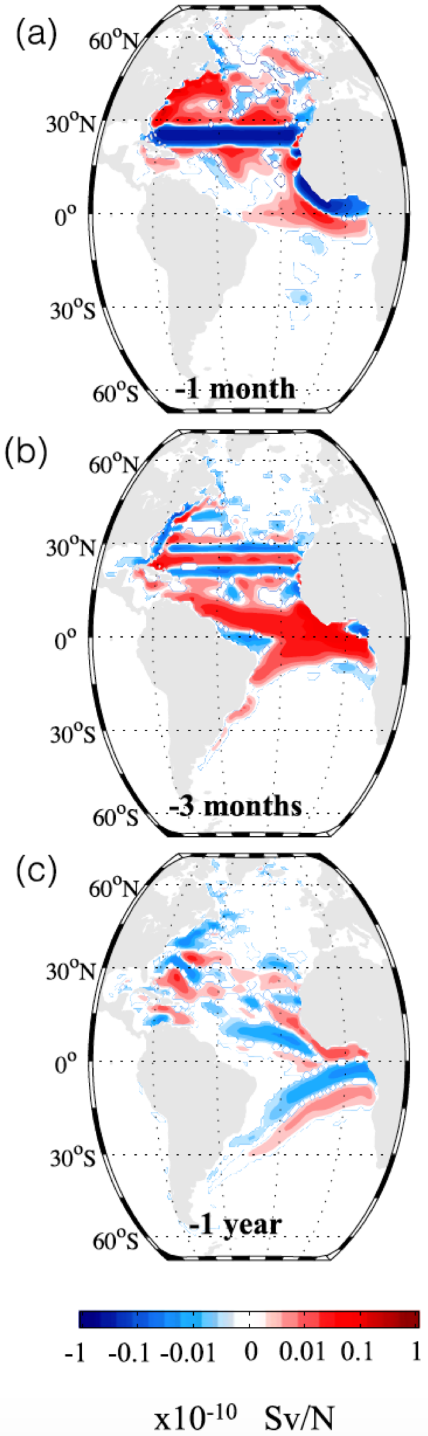
$$\frac{\partial J}{\partial x_0} = \sum_{1\le k\le N} \frac{\partial x_k}{\partial x_0}\left(\frac{\partial J}{\partial x_k}\right)$$

$$= \frac{\partial x_1}{\partial x_0}\left(\frac{\partial J}{\partial x_1}\right) + \frac{\partial x_1}{\partial x_0}\frac{\partial x_2}{\partial x_1}\left(\frac{\partial J}{\partial x_2}\right) + \ldots + \frac{\partial x_1}{\partial x_0}\cdots\frac{\partial x_N}{\partial x_{N-1}}\left(\frac{\partial J}{\partial x_N}\right)$$

Dynamical attribution:
The Atlantic MOC @ 26°N

Sensitivity of *J*
with respect to
zonal wind stress,
1, 3, and 12 months
back in time,
…
carried by the
time-evolving
dual/adjoint state

Pillar et al., J. Clim. (2016)



Recall:

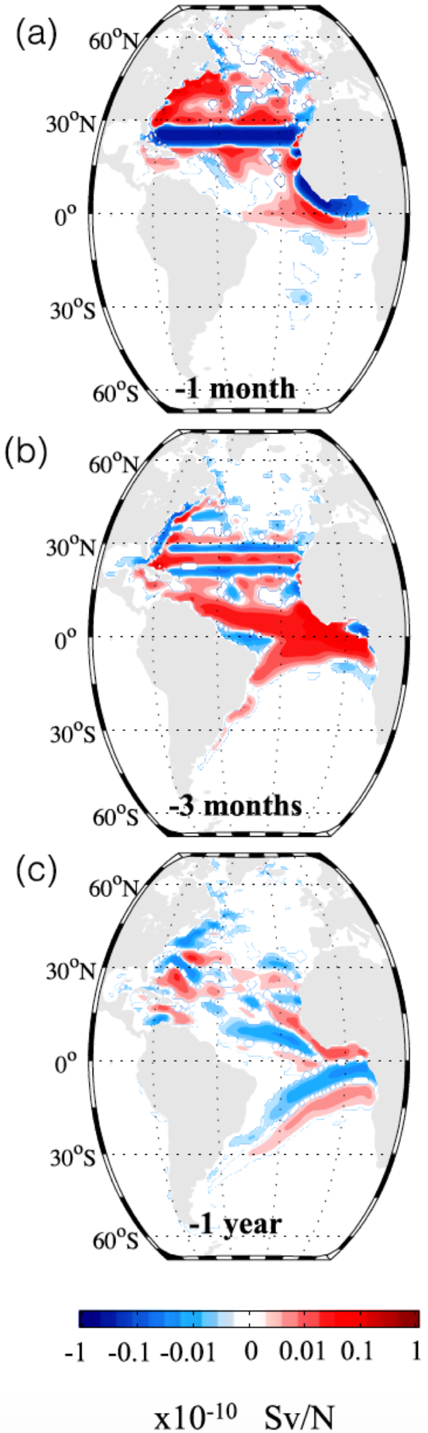
$$\frac{\partial J}{\partial x_0} = \sum_{1\leq k\leq N} \frac{\partial x_k}{\partial x_0} \left(\frac{\partial J}{\partial x_k} \right)$$

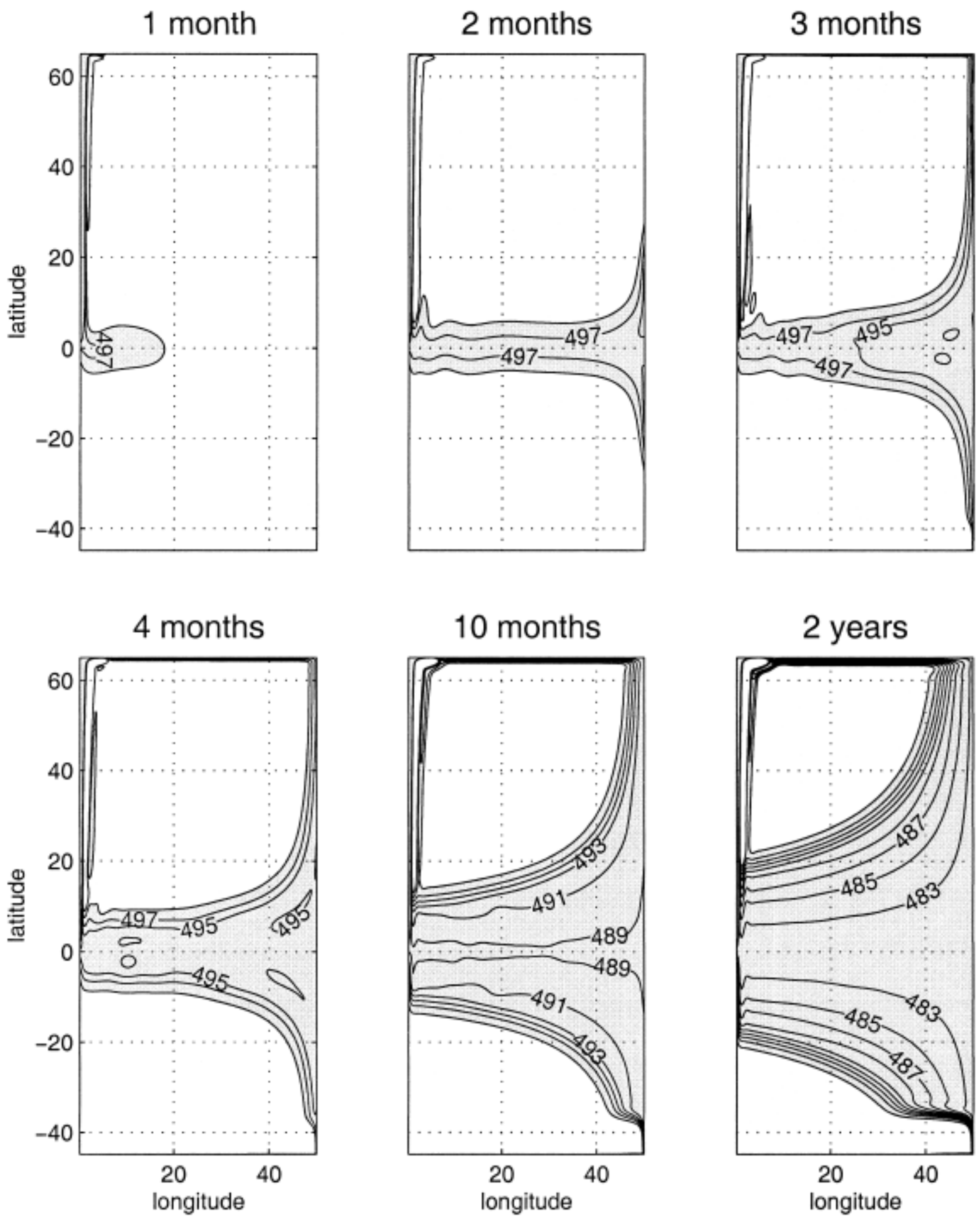
$$= \frac{\partial x_1}{\partial x_0} \left(\frac{\partial J}{\partial x_1} \right) + \frac{\partial x_1}{\partial x_0} \frac{\partial x_2}{\partial x_1} \left(\frac{\partial J}{\partial x_2} \right) + \ldots + \frac{\partial x_1}{\partial x_0} \cdots \frac{\partial x_N}{\partial x_{N-1}} \left(\frac{\partial J}{\partial x_N} \right)$$

Dynamical attribution:
The Atlantic MOC @ 26°N

Sensitivity of *J*
with respect to
zonal wind stress,
1, 3, and 12 months
back in time,
…
carried by the
time-evolving
dual/adjoint state

Pillar et al., J. Clim. (2016)



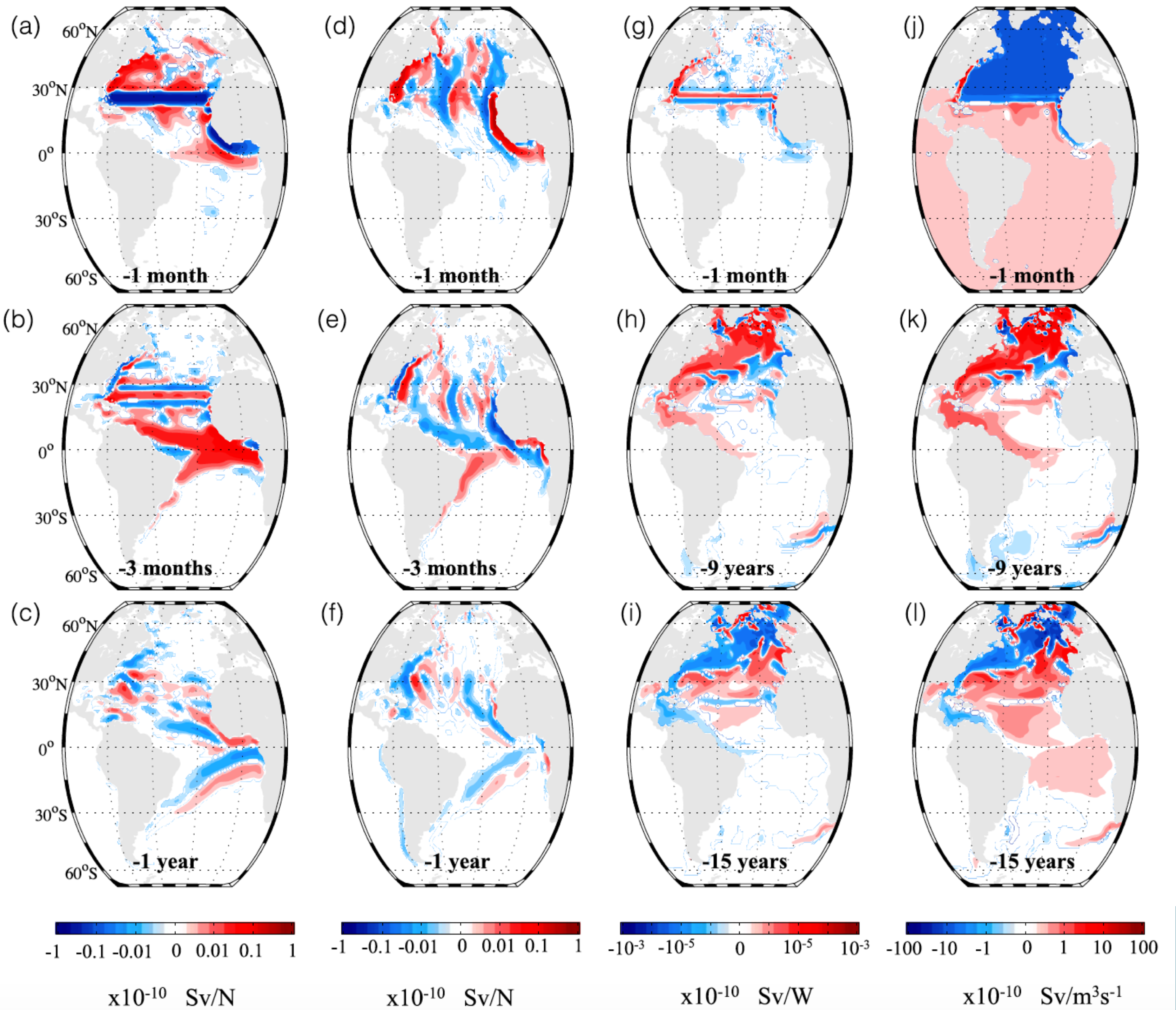


H. Johnson & D. Marshall (2002)

Dynamical attribution:
The Atlantic MOC @ 26°N

Sensitivity of *J*
with respect to
(**from left to right**):

- zonal wind stress
- merid. wind stress
- heat flux
- freshwater flux



Pillar et al., J. Clim. (2016)

Dynamical attribution:
The Atlantic MOC @ 26°N

(Where) are uncertainties in externally forced AMOC uncertainties determined by …

1. **regions most sensitive to forcings?**
2. **regions exhibiting largest forcing uncertainties?**

$$\delta\mathcal{J}(t) = \sum_{k}^{N_{atm}} \delta\mathcal{J}_k(t)$$
$$= \sum_{k}^{N_{atm}} \int_{t_0}^{t} \int_x \int_y \frac{\partial\mathcal{J}}{\partial u_k}(x, y, \tau - t_f)\, \delta u_k(x, y, \tau)\, dxdyd\tau$$

Dynamical attribution:

The Atlantic MOC

$$\boxed{\frac{\partial \mathcal{J}}{\partial u_k}}$$

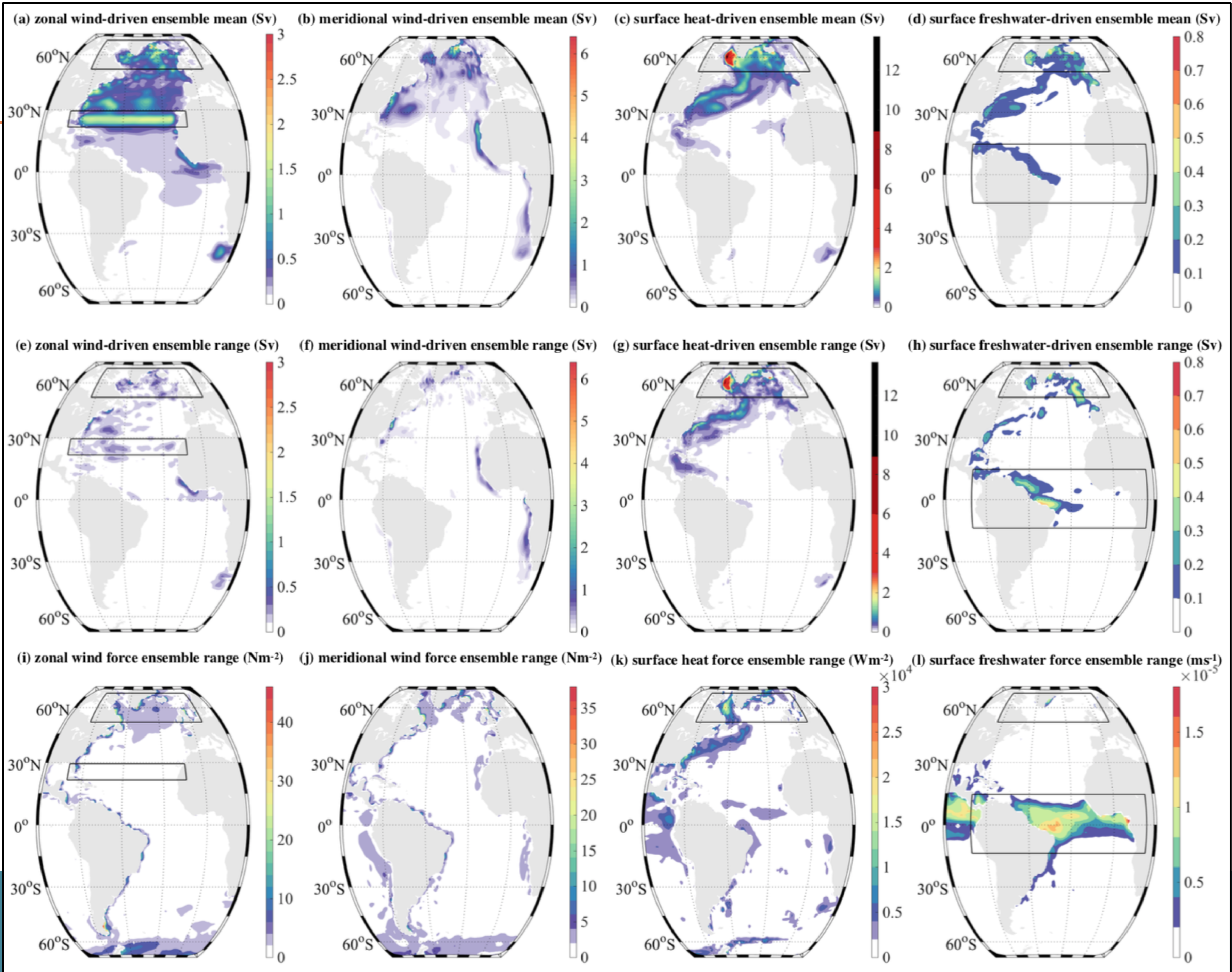
$$\Downarrow$$

$$\delta \mathcal{J}_k(t)$$

$$\Uparrow$$

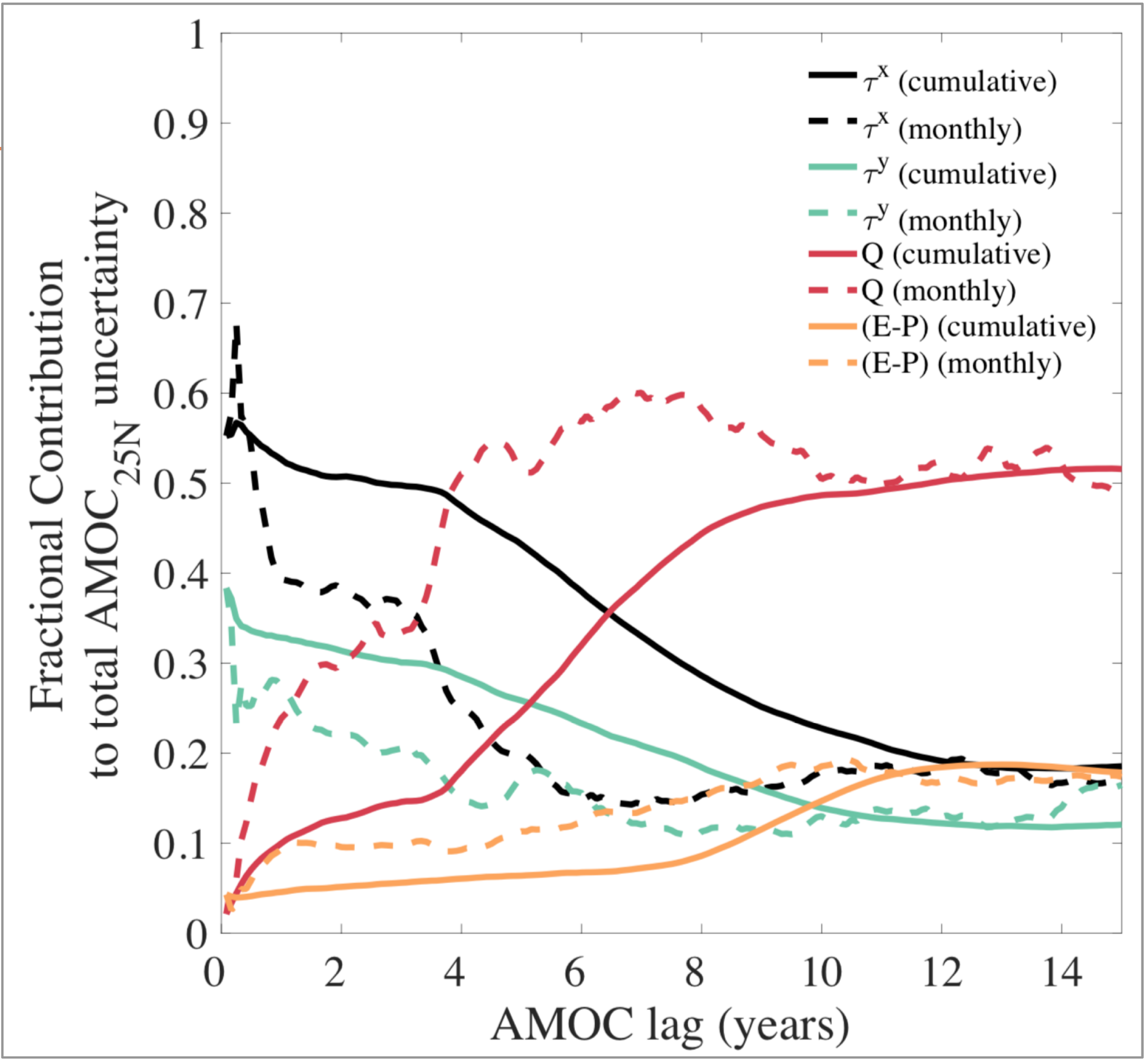
$$\boxed{\delta u_k(x, y, \tau)}$$

Pillar et al., J. Clim. (2018)



Dynamical attribution:
The Atlantic MOC @ 26°N

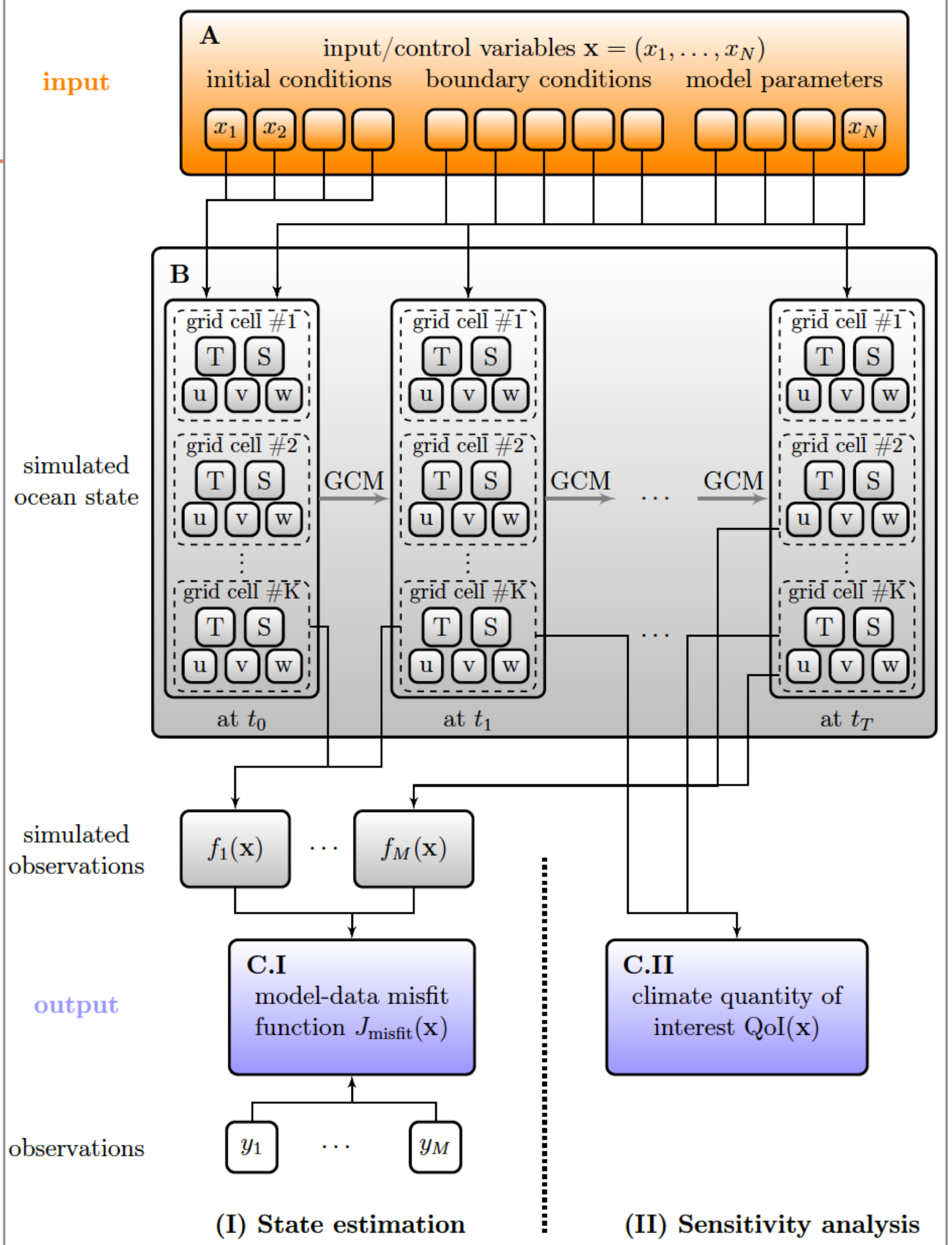
Fractional contribution of uncertainty in reanalysis air-sea flux forcing fields to the total uncertainty in the modelled AMOC



Pillar et al., J. Clim. (2018)

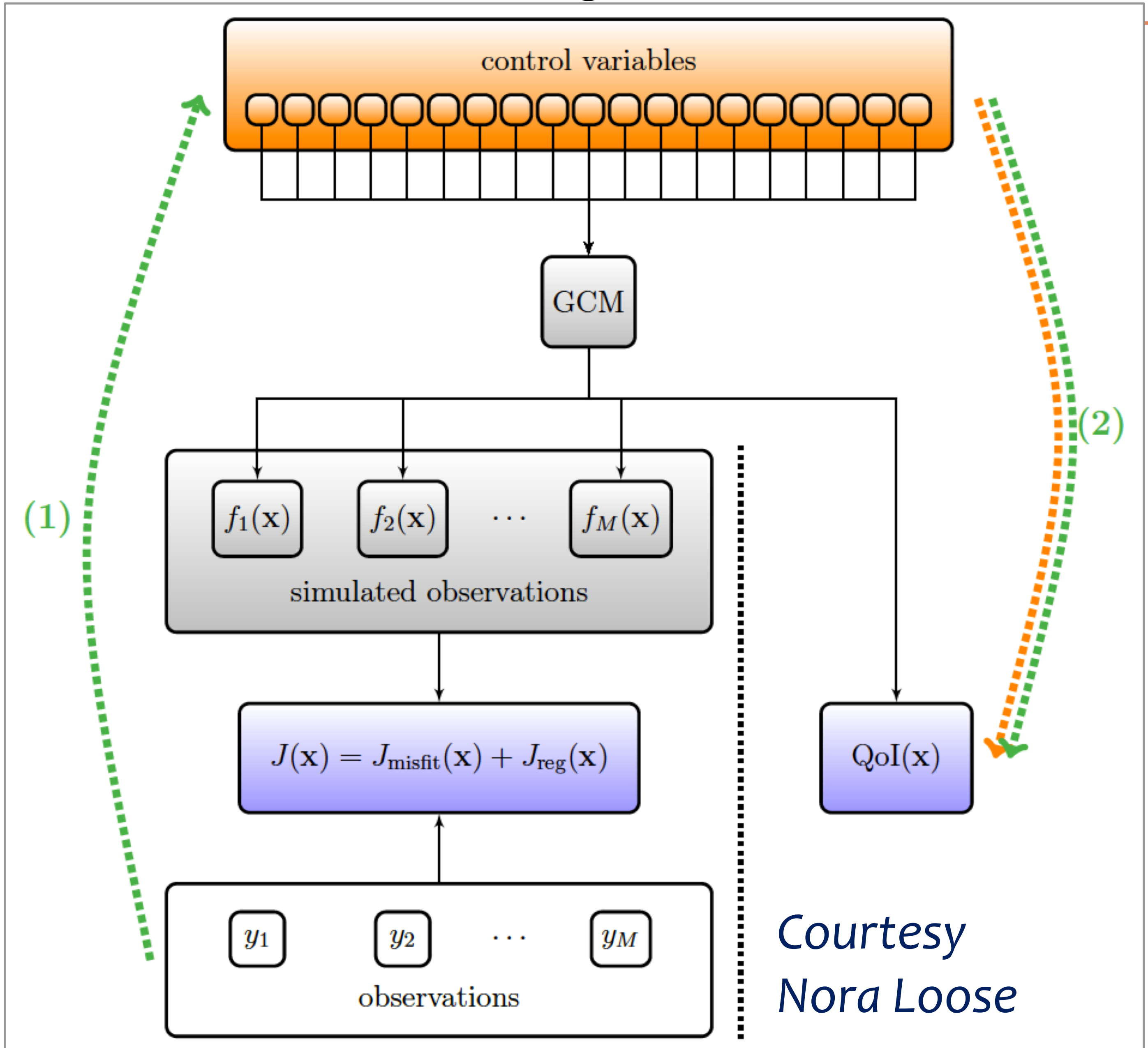
4.
Uncertainty Quantification & Optimal Observing System Design

Recall:
The inverse problem

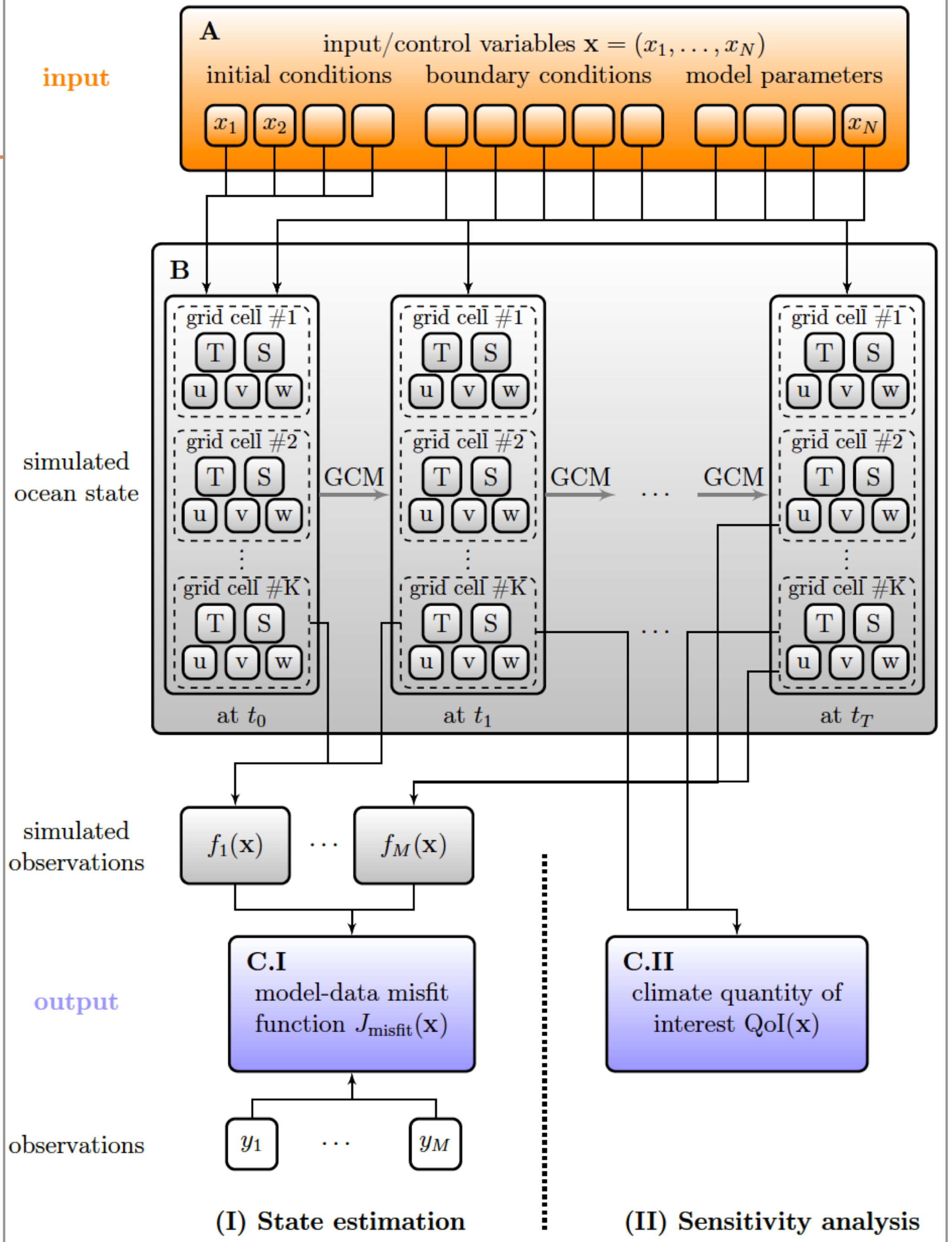


Courtesy
Nora Loose

Now:
The uncertainty propagation problem



Courtesy Nora Loose



More on this on Thursday AM

Uncertainty reduction of QoI $\mathcal{Q}$ through observation $\mathcal{J}$

$$1 - \frac{\mu_{post}}{\mu_{prior}} = d_1 \left\langle \frac{B^{1/2}\left(\frac{\partial \mathcal{Q}}{\partial x}\right)^T}{\|B^{1/2}\left(\frac{\partial \mathcal{Q}}{\partial x}\right)^T\|}, \frac{B^{1/2}\left(\frac{\partial \mathcal{J}}{\partial x}\right)^T}{\|B^{1/2}\left(\frac{\partial \mathcal{J}}{\partial x}\right)^T\|} \right\rangle$$

$$= d_1 < \text{info required by } \mathcal{Q}, \text{ info transmitted by } \mathcal{J} >$$

Nora Loose (Uni Bergen & Oden Institute), Ph.D. thesis (2019)

Looking beyond optimization…

- Adjoints are powerful tool for gaining dynamical and quantitative insight into processes governing ocean variability
  - (linear) sensitivity analysis
  - dynamical (as opposed to statistical) attribution
  - non-normal transient amplification (not shown)
  - uncertainty quantification
  - optimal observing system design
  - …
- Plenty of reasons for exploring adjoint models