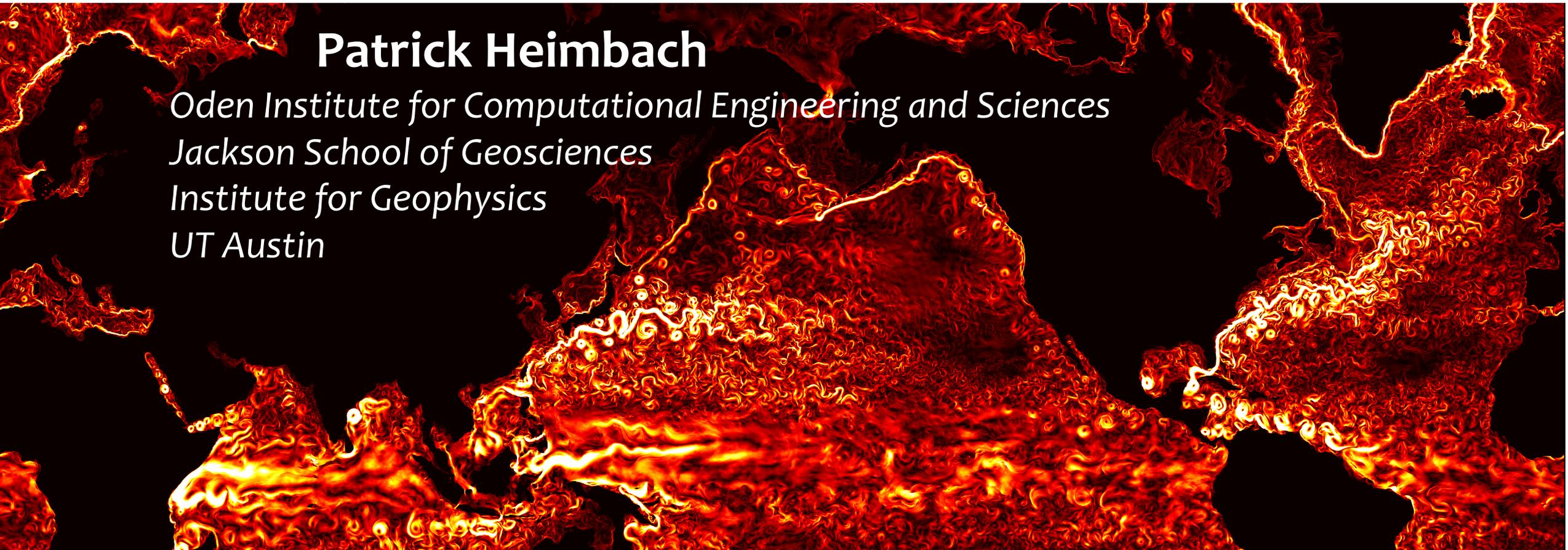


Learning from sparse observations: The global ocean state and parameter estimation problem

Patrick Heimbach

*Oden Institute for Computational Engineering and Sciences
Jackson School of Geosciences
Institute for Geophysics
UT Austin*





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Remi Tailleux @RemiTailleux · 17h



In traditional physics, theoreticians predict how observable quantities should behave should their theory be correct. In physical oceanography, however, theoreticians most often do the opposite, e.g, they use observations to predict non-observable quantities. **Can we do better?**

 2

 1

 5



Can we do better?

**Realistically, probably not much in the near future,
if by “better” you mean a drastic improvement
of observational capabilities.**

BUT, ... enter Computational Science and Engineering:

It is an essential driving force for progress in science
in applications where experimental / observational approaches are ...

- *too costly,*
- *too slow,*
- *dangerous,*
- *or impossible*

SIAM REVIEW
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Research and Education in Computational Science and Engineering*

Officers of the SIAM Activity Group on Computational Science and
Engineering (SIAG/CSE), 2013–2014:

Ulrich Rüde[†]

Karen Willcox[‡]

Lois Curfman McInnes[§]

Hans De Sterck[¶]

Computational Science and Engineering @ the Oden Institute

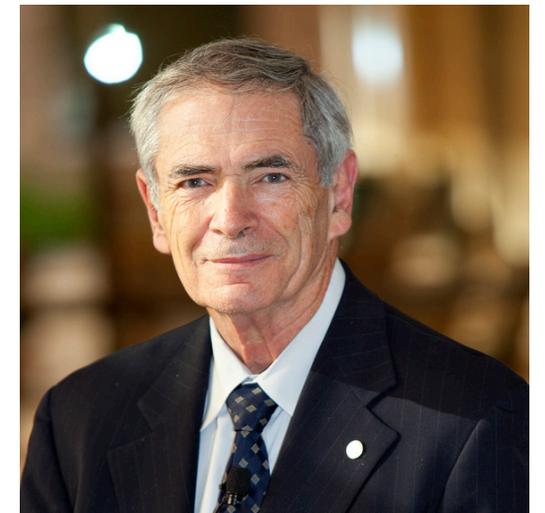
- In particular, CSE offers tools for addressing optimal observing design:
- When a quantity of interest (QoI) is unobserved (different variable or different location, or both – an ubiquitous problem) ...
 - What is an optimal sampling strategy with given observational assets to best constrain the QoI?

Predictive Computational Science: Computer Predictions in the Presence of Uncertainty

J. Tinsley Oden, Ivo Babuska, and Danial Faghihi

*Institute for Computational Engineering and Sciences
The University of Texas at Austin*

oden@ices.utexas.edu, babuska@ices.utexas.edu, danial@ices.utexas.edu.



1. The global ocean circulation – a *big* or *sparse data* problem?
2. The global ocean circulation as an *inverse problem*
 - Optimal estimation for calibration & reconstruction
3. Causal / dynamical attribution based on the *dual* ocean state
4. UQ in large-scale inverse problems based on *Hessians*
 - Optimal experimental (observing system) design

1.

The global ocean circulation:

A big & sparse data problem

Is Oceanography a Big Data Science?

Is Oceanography a Big Data Science?

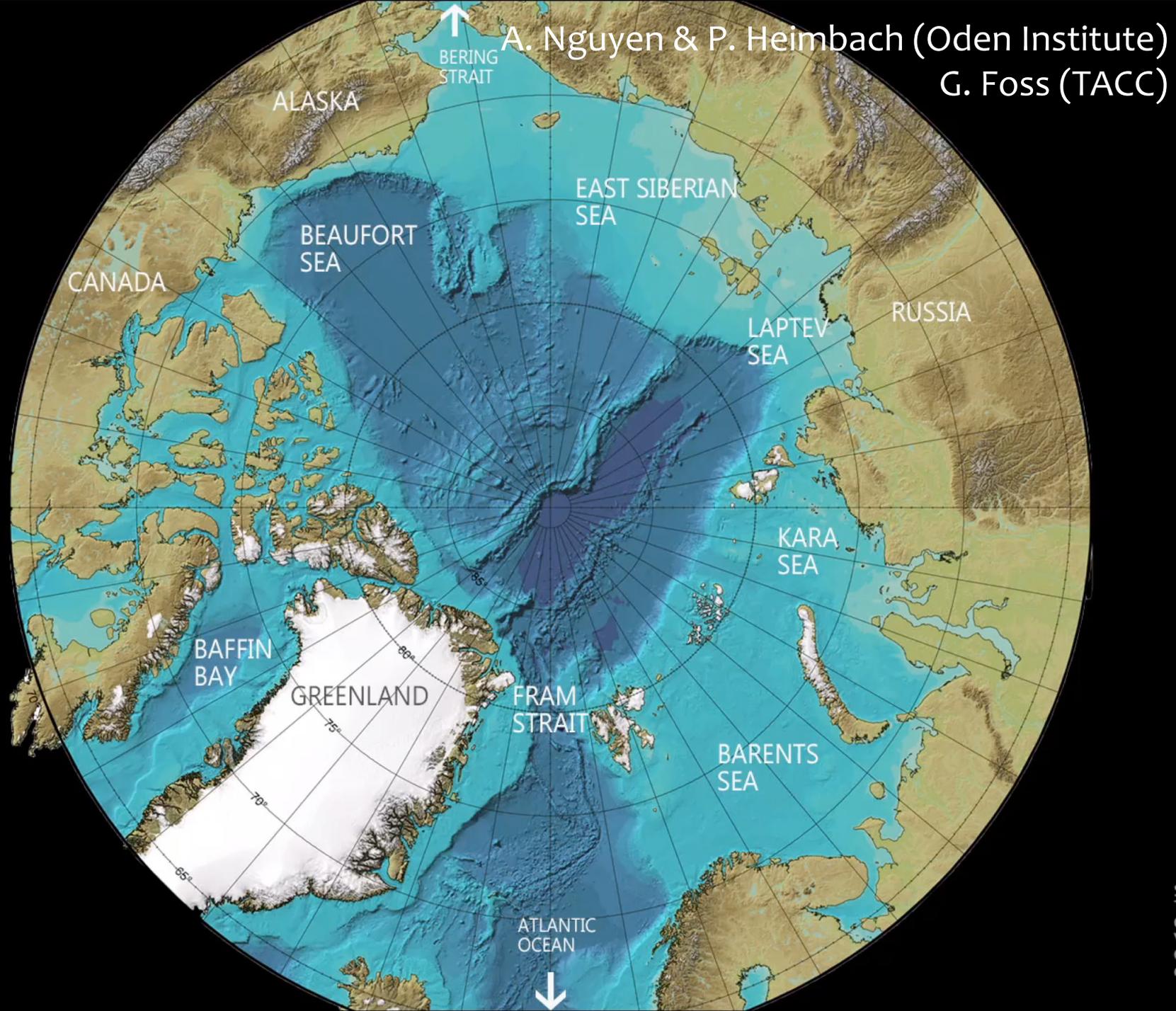
YES, you might say...

Prelude

- Simulating the coupled climate system with increasing
 - detail (resolution)
 - complexity (process representation)
- creates vast output

Example:

Simulation of Arctic Ocean subsurface circulation at eddy-permitting resolution



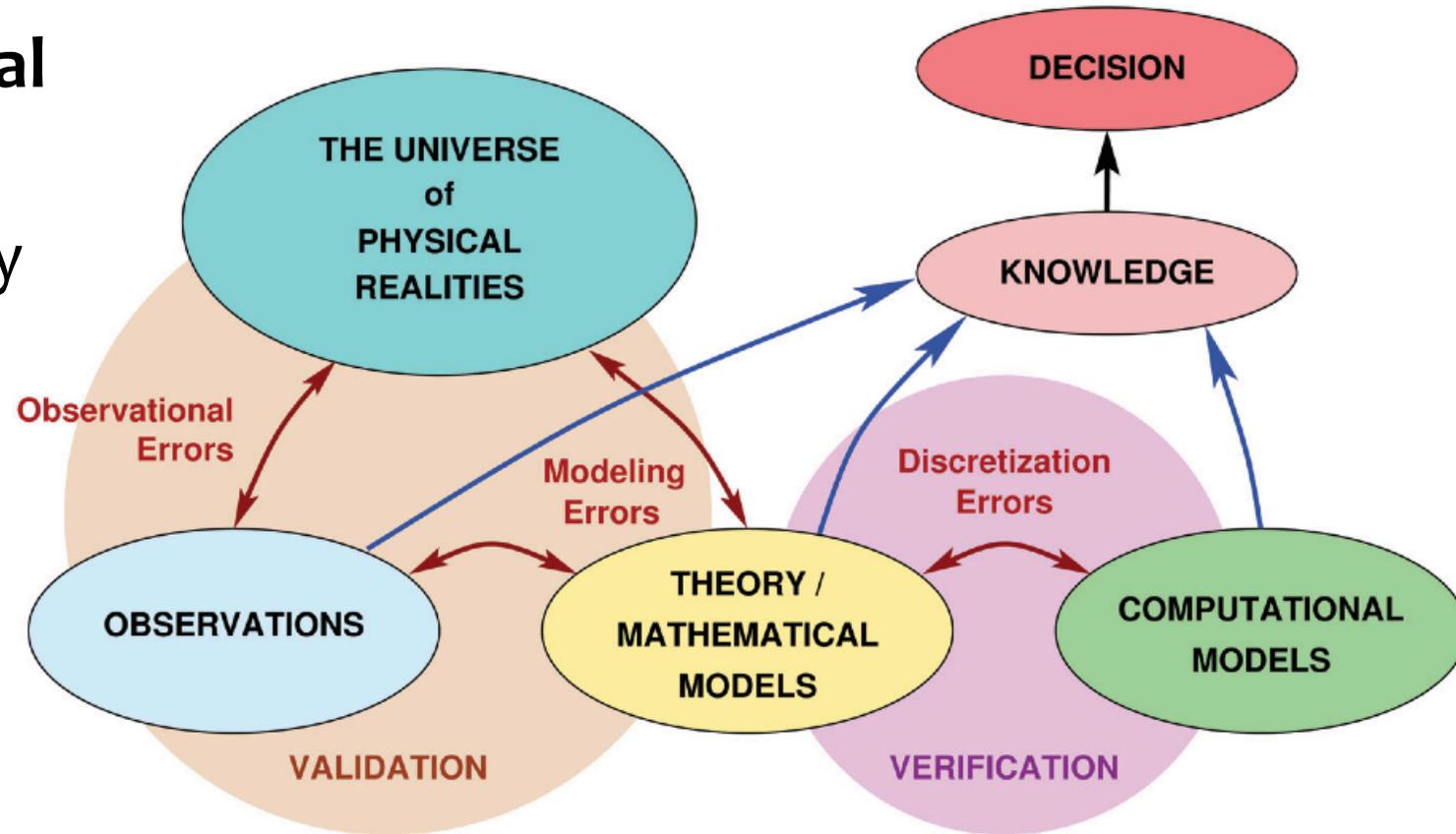
Simulations ...

... give access to detailed phenomena of the time evolving state of the ocean that is consistent with our theoretical knowledge (i.e., equations of motions)

BUT ...

... significant uncertainties remain

- **Constitutive laws are empirical**
 - uncertain structure & parameters (and which may vary in 3+1-dim.)
- **Discretization requires numerical approximation & parameterization**
 - e.g.: related to surface and bottom-intensified mixing
- **Uncertain external forcings**



Oden, Moser, Ghattas, SIAM News (2010)

Prelude

- How realistic are our simulations?
- What aspects of the simulations are robust?
- How do errors accumulate over time and space?
 - Are they acceptably bounded?
 - How to quantify?

**We need observations to ground theory & simulation,
even with improved model resolution & process representation**

Is Oceanography a Big Data Science?

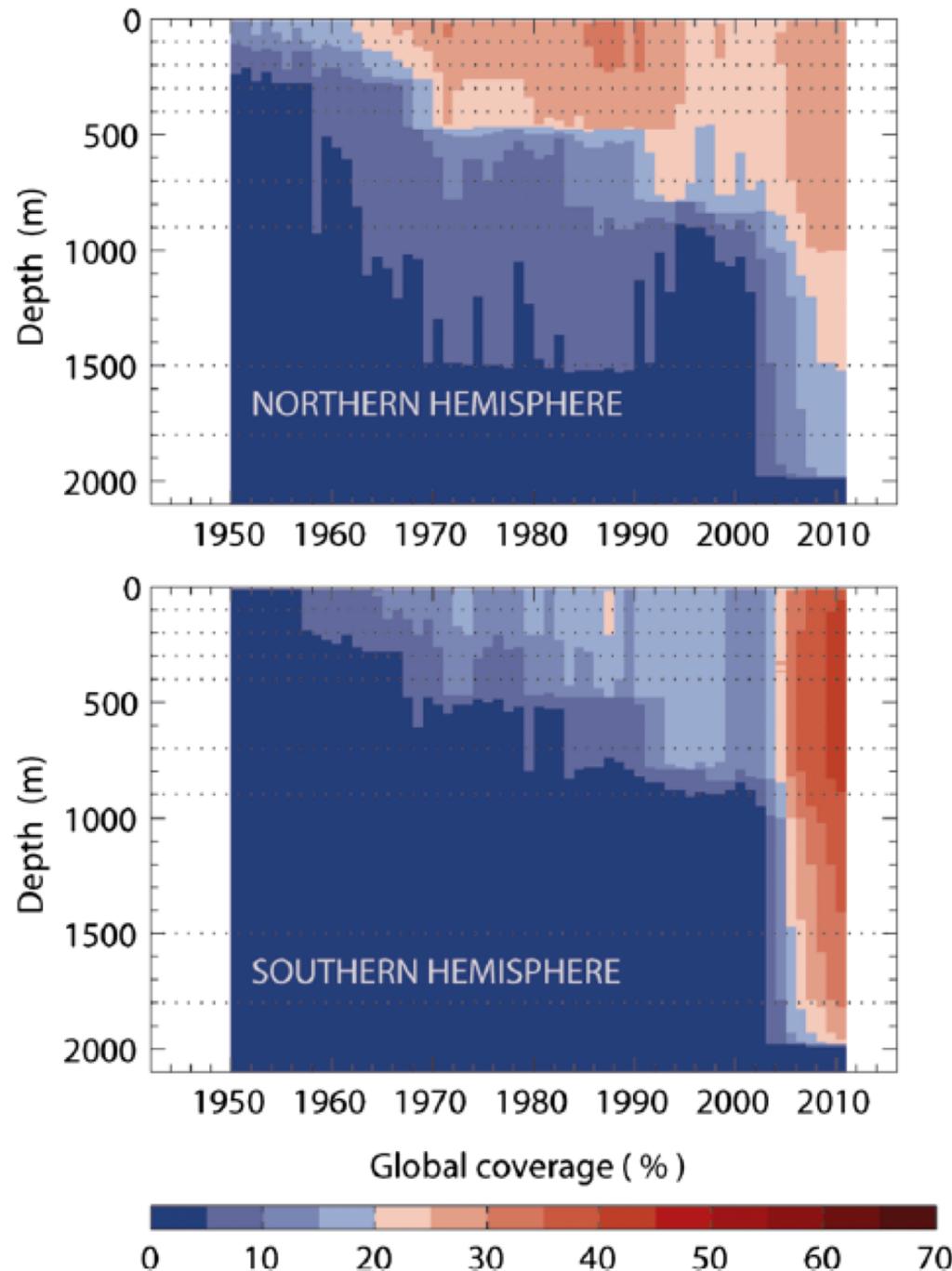
Is Oceanography a Big Data Science?

NO, you might say...

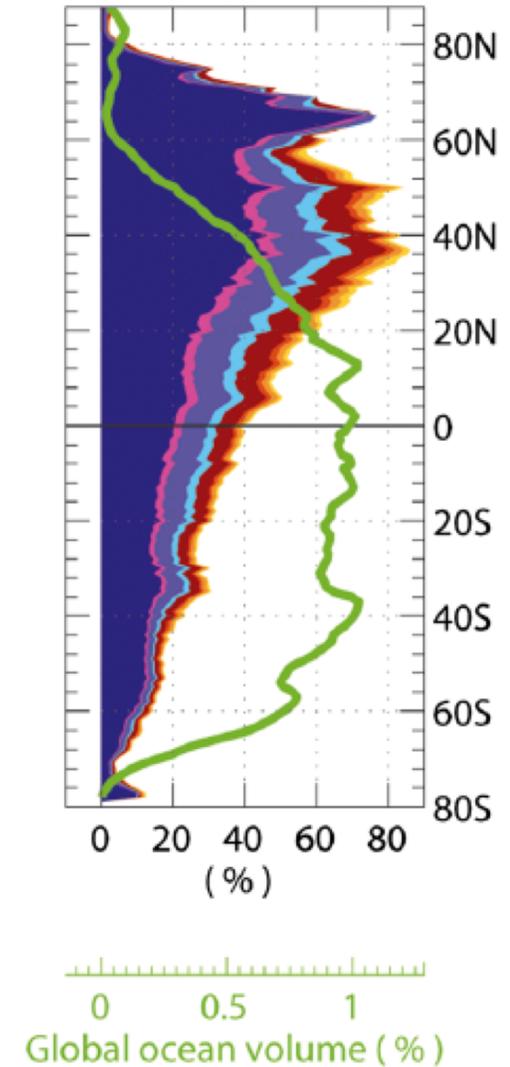
Some of the challenges:
Sparse sampling of the ocean's

Observational sampling
coverage for ocean
temperature in the
upper 2000 m

Abraham et al., Rev. Geophys. (2013)

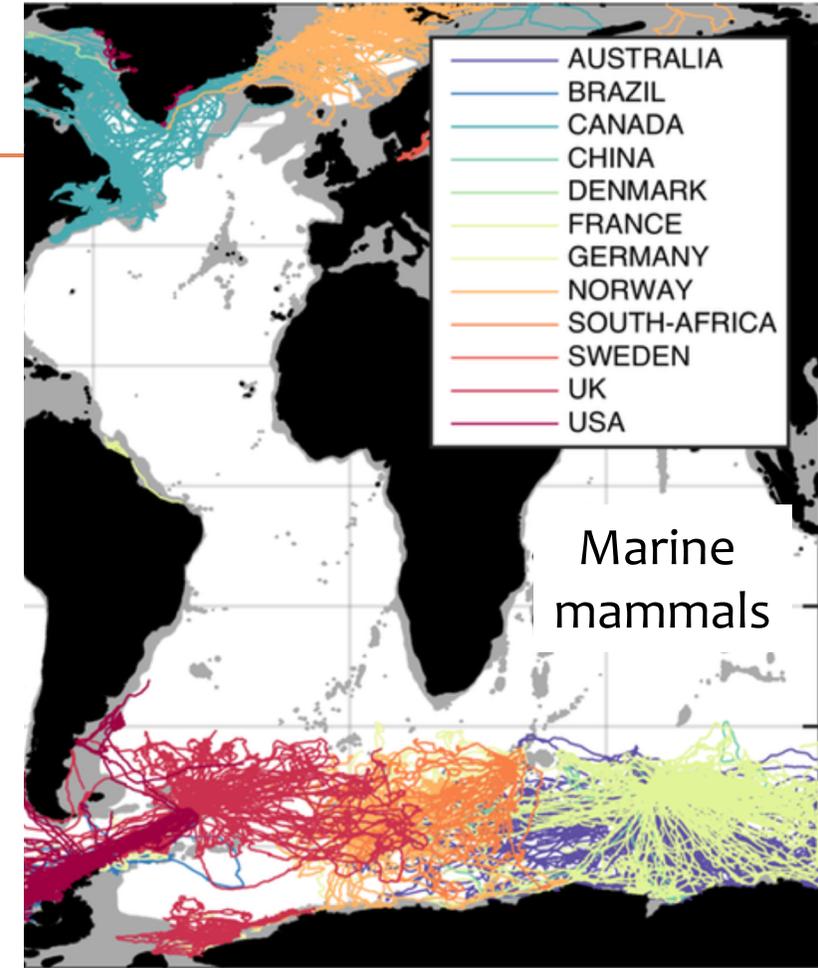
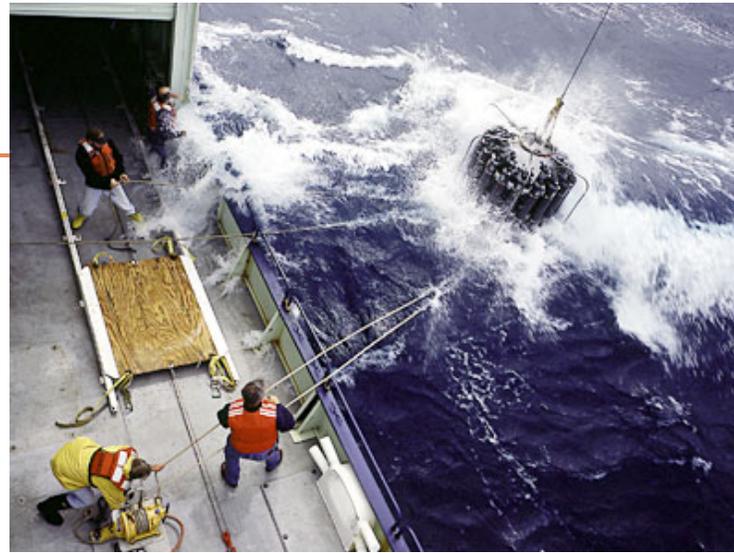


Mean zonal coverage
(1950–2011)

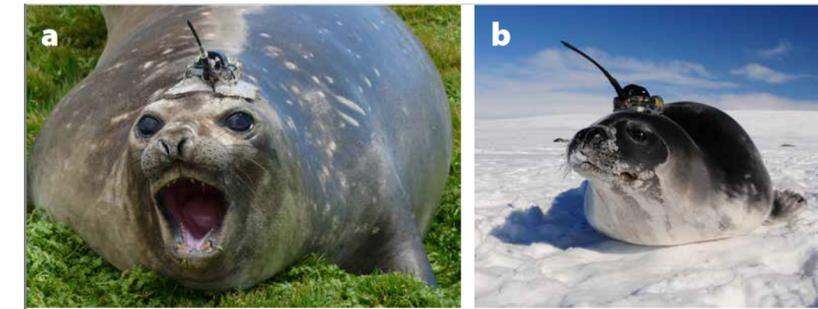
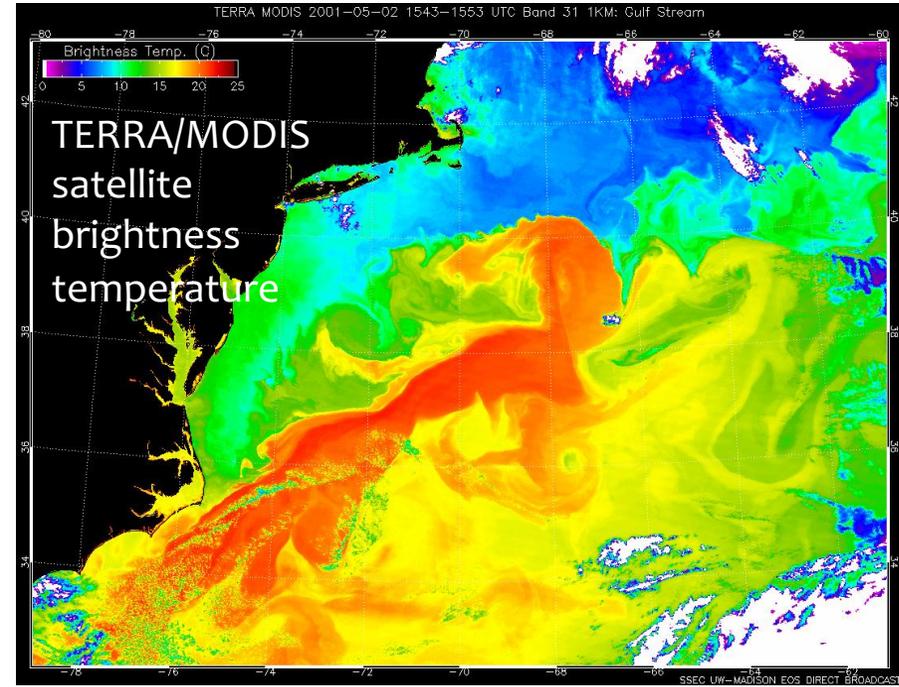
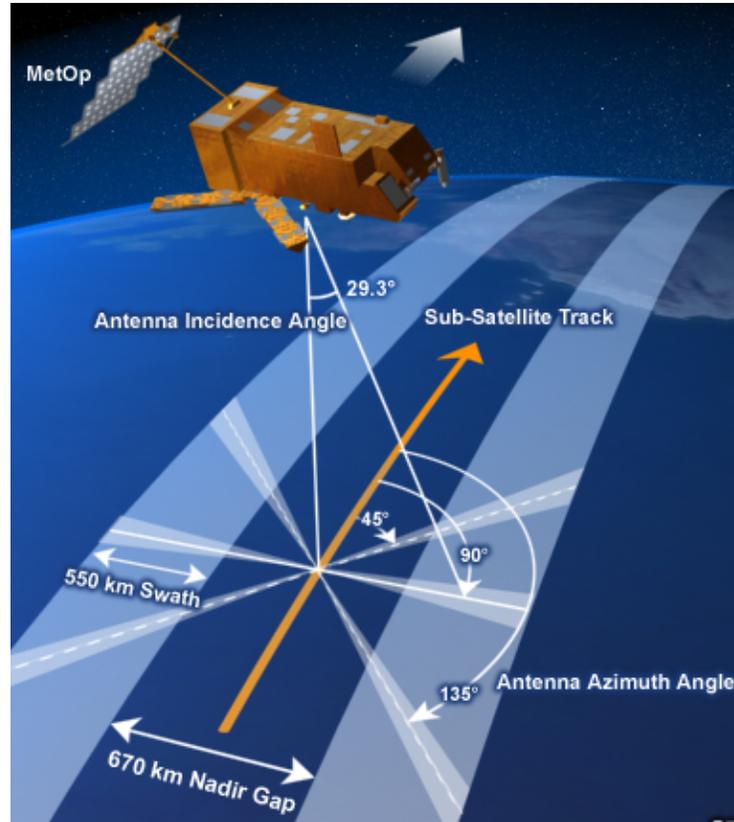


(colors refer to
depth ranges)

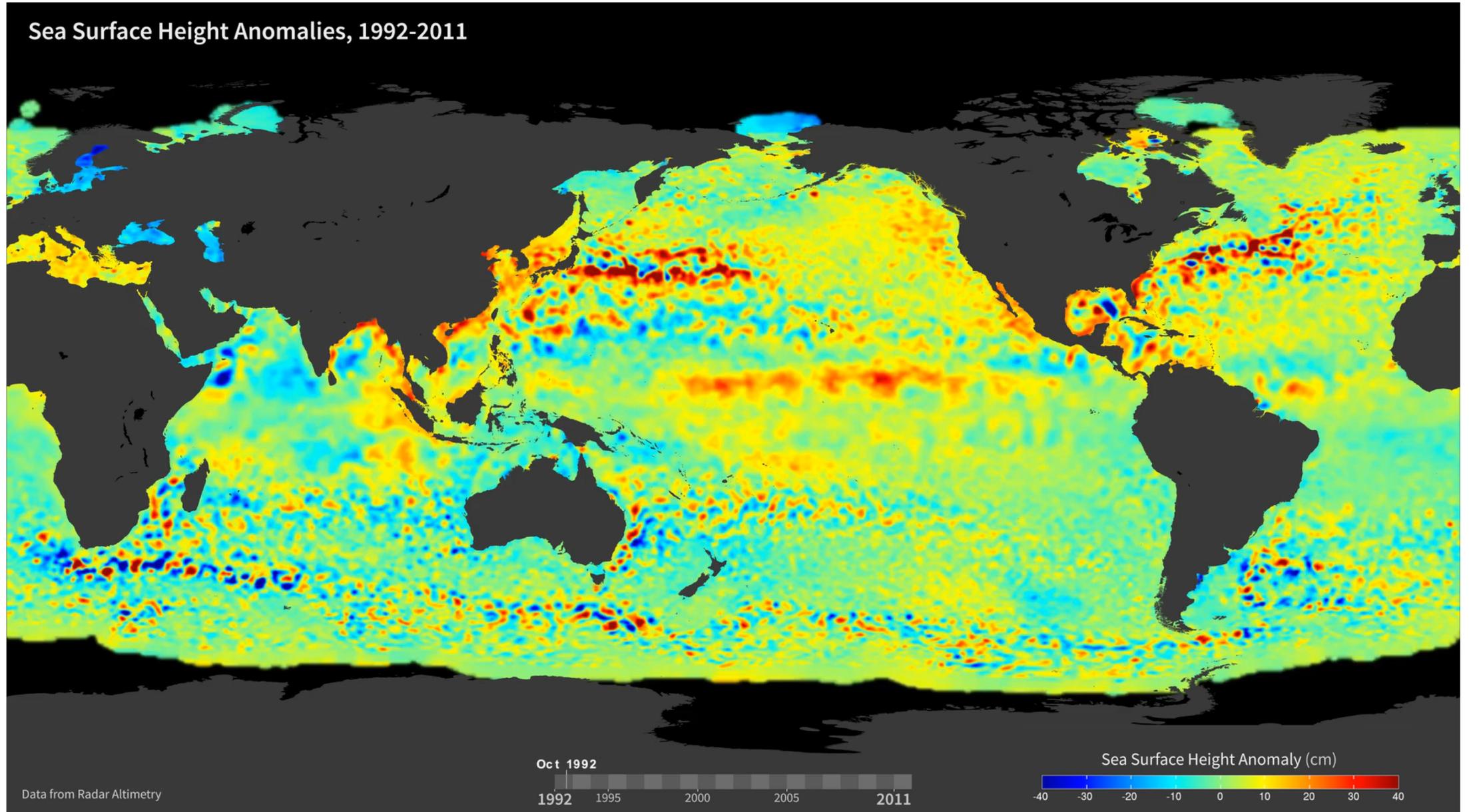
Some of the challenges: Disparate data streams



<http://www.meop.net>



An eclectic global ocean observing system in a “noisy” ocean



An eclectic global ocean observing system ...
... in a “noisy” ocean

- Heterogeneous data streams
- Disparate variables being sampled
- Spatio-temporally non-uniform sampling
- ...

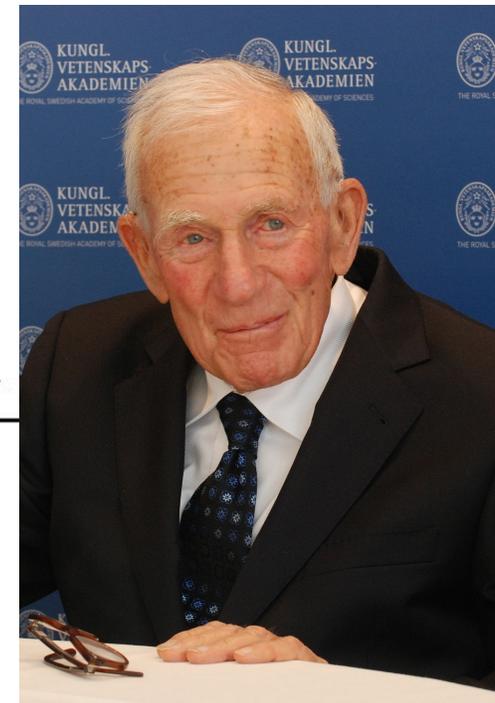
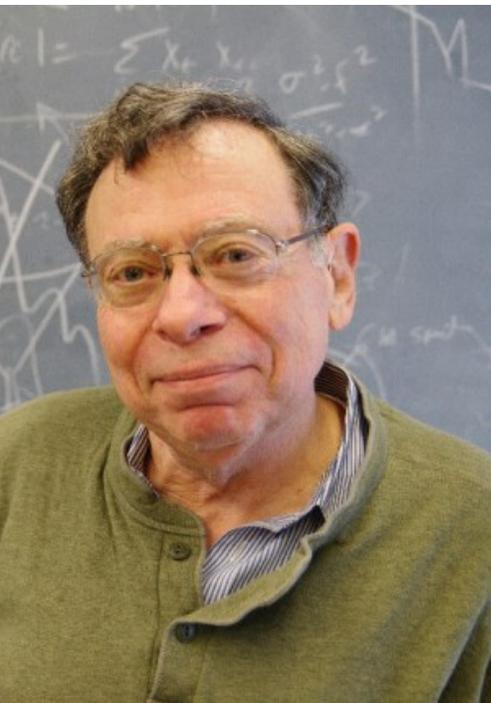
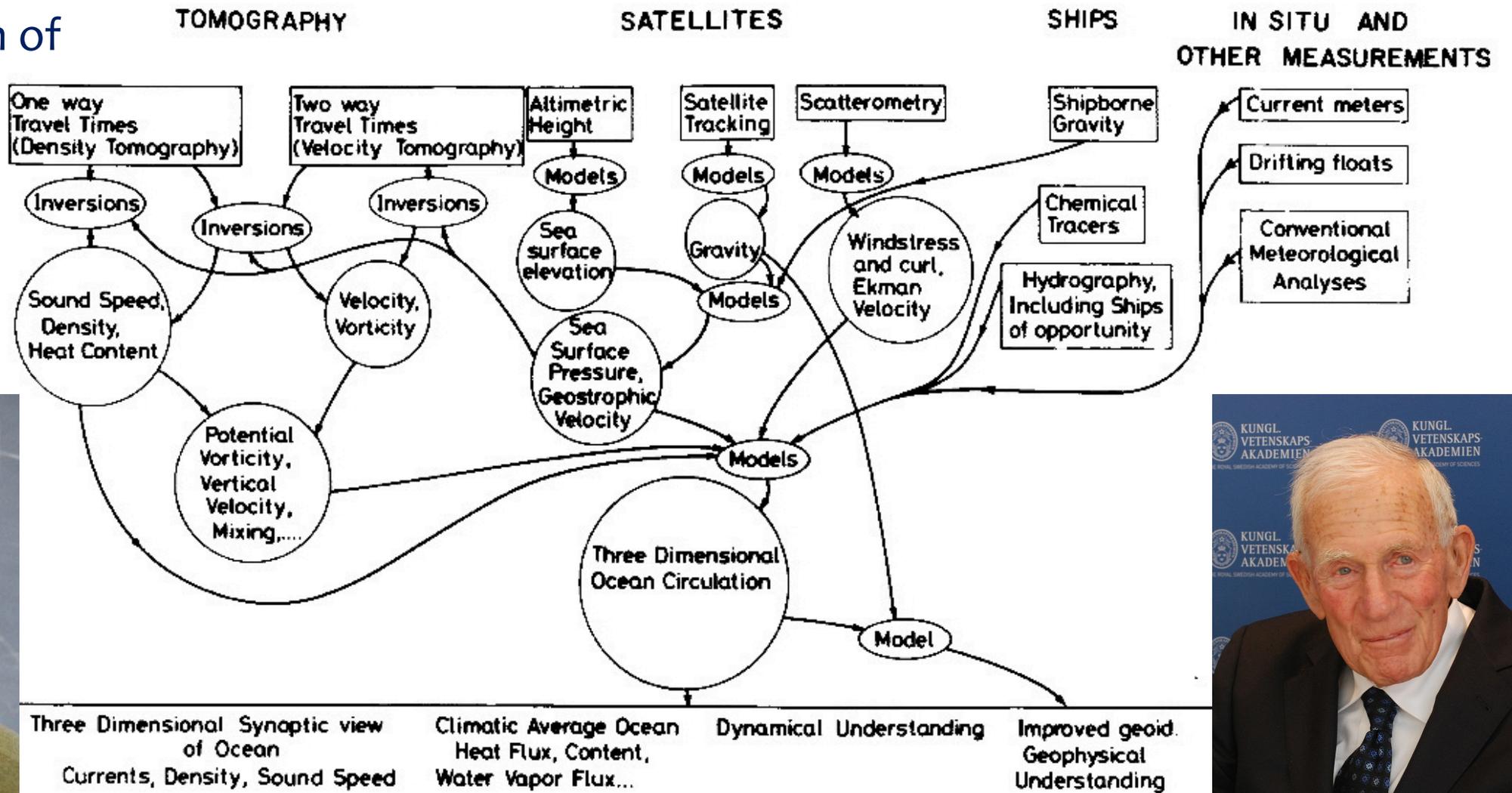
**How best to synthesize the information
contained in the data into a single framework?**

2.

The global ocean circulation inverse problem

The ocean circulation inverse problem – historical

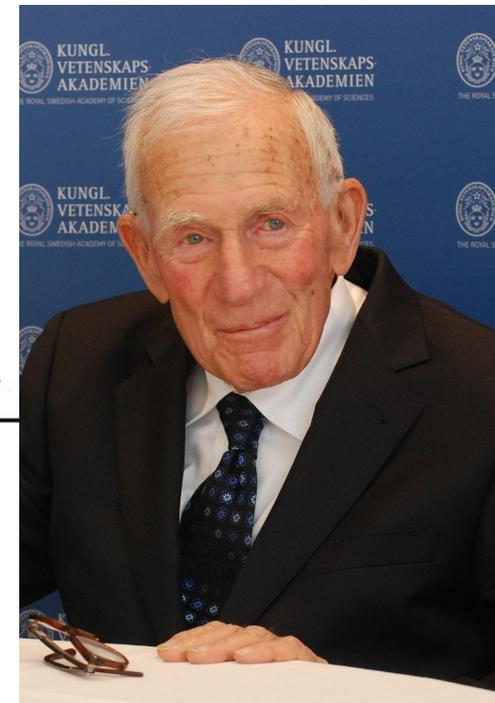
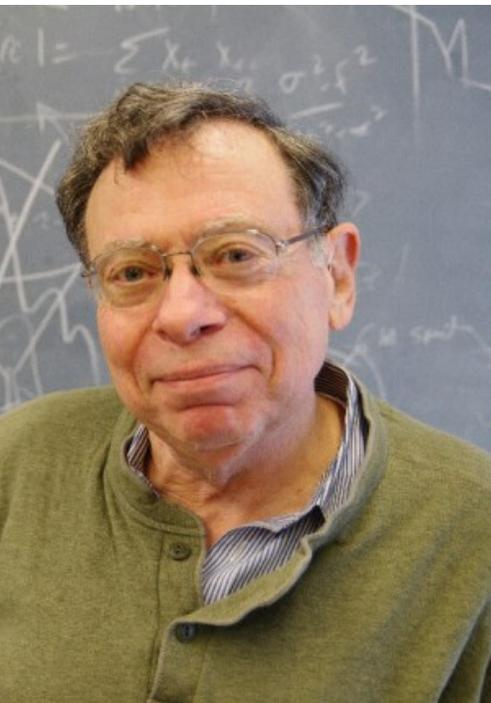
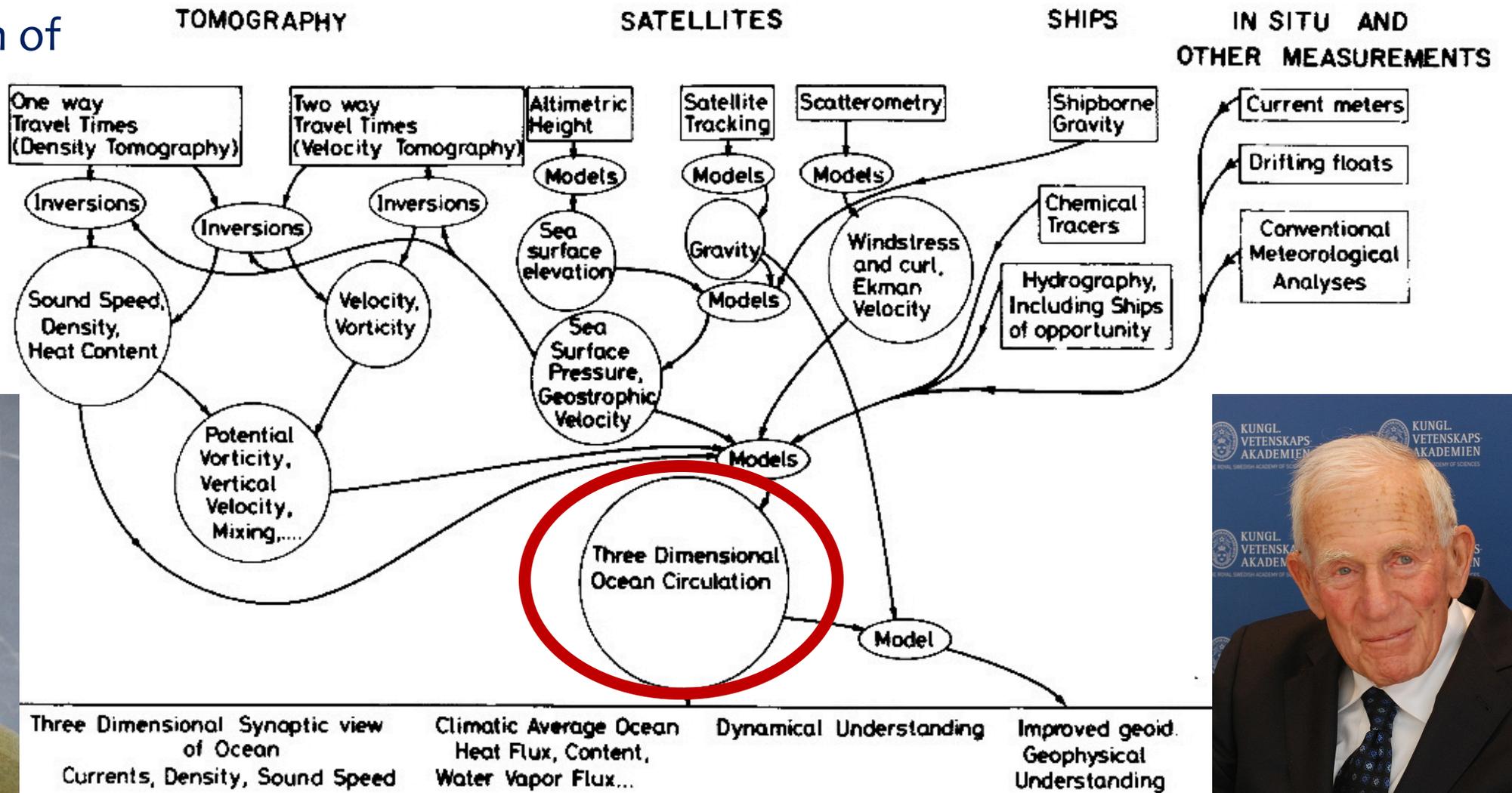
On the occasion of
Walter Munk's
65th Birthday
Symposium
1982



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

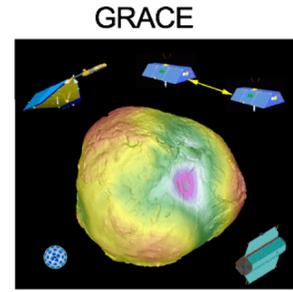
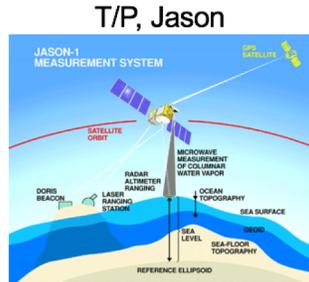
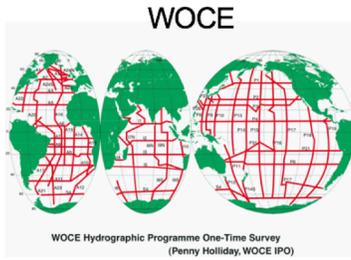
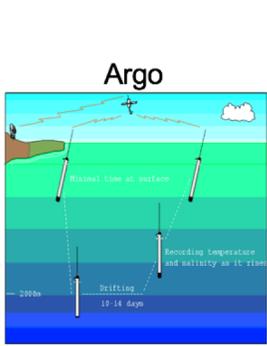
The ocean circulation inverse problem – historical

On the occasion of
Walter Munk's
65th Birthday
Symposium
1982



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

The ocean circulation inverse problem – today

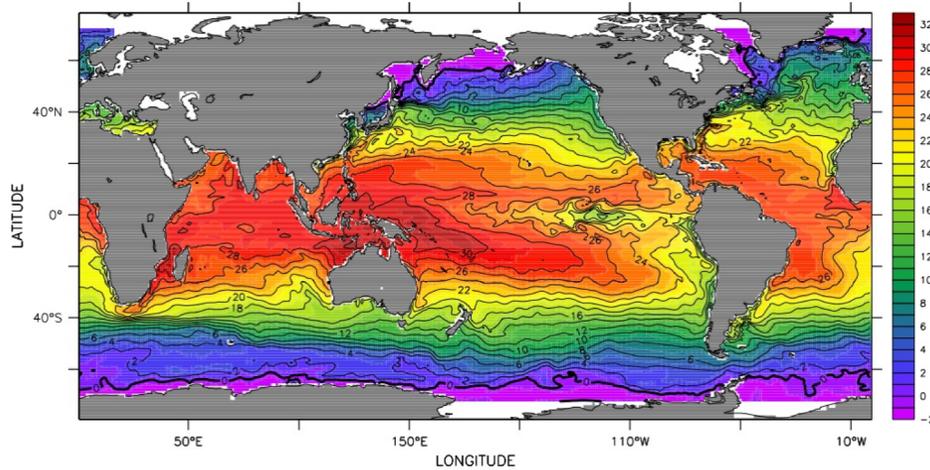


How to synthesize? Estimation/optimal control problem:
Use a **model** (MITgcm) and its **adjoint**:

DEPTH (m) : 5
TIME : 01-JAN-2000 00

DATA SET: Tave

Assimilation (Adjoint) by ODAP



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

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

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

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

$$\frac{D\theta}{Dt} = Q_\theta$$

$$\frac{DS}{Dt} = Q_s$$



- Stammer et al., JGR (2002)
- Wunsch & Heimbach, Physica D (2007)

The ocean circulation inverse problem – today

Very brief review and
example science
applications

Heimbach et al.
Front. Mar. Sci. (2019)

Putting It All Together: Adding Value to the Global Ocean and Climate Observing Systems With Complete Self-Consistent Ocean State and Parameter Estimates

Patrick Heimbach^{1,2,3}, Ichiro Fukumori⁴, Christopher N. Hill⁵, Rui M. Ponte⁶, Detlef Stammer⁷, Carl Wunsch^{5,8}, Jean-Michel Campin⁵, Bruce Cornuelle⁹, Ian Fenty⁴, Gaël Forget⁵, Armin Köhl⁷, Matthew Mazloff⁹, Dimitris Menemenlis⁴, An T. Nguyen¹, Christopher Piecuch¹⁰, David Trossman¹, Ariane Verdy⁹, Ou Wang⁴ and Hong Zhang⁴*

¹ Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX, United States, ² Institute for Geophysics, The University of Texas at Austin, Austin, TX, United States, ³ Jackson School of Geosciences, The University of Texas at Austin, Austin, TX, United States, ⁴ Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, United States, ⁵ Department of Earth, Atmospheric, and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, MA, United States, ⁶ Atmospheric and Environmental Research, Lexington, MA, United States, ⁷ Center für Erdsystemforschung und Nachhaltigkeit, Universität Hamburg, Hamburg, Germany, ⁸ Department of Earth and Planetary Sciences, Harvard University, Cambridge, MA, United States, ⁹ Scripps Institution of Oceanography, La Jolla, CA, United States, ¹⁰ Department of Physical Oceanography, Woods Hole Oceanographic Institution, Woods Hole, MA,

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:

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

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

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

The ocean circulation inverse problem

Lagrange multiplier method:

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

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}(t)} = \mathbf{x}(t) - L[\mathbf{x}(t-1)] = 0 \quad 1 \leq t \leq t_f$$

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

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}(t_f)} = \frac{\partial J}{\partial \mathbf{x}(t_f)} - \boldsymbol{\mu}(t_f) = 0 \quad t = t_f$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{x}(0)} = \frac{\partial J}{\partial \mathbf{x}(0)} - \left[\frac{\partial L[\mathbf{x}(0)]}{\partial \mathbf{x}(0)} \right]^T \boldsymbol{\mu}(1) \quad t_0 = 0$$

The ocean circulation inverse problem

For intermediate step of the adjoint model integration one obtains:

$$\begin{aligned}\mu_k &= \frac{\partial J}{\partial x_k} = \mathbf{L}^T \frac{\partial J}{\partial x_{k+1}} + \mathbf{E}^T \mathbf{R}^{-1} [\mathbf{E}x_k - y_k] \\ &= \mathbf{L}^T \left(\mathbf{L}^T \frac{\partial J}{\partial x_{k+2}} + \mathbf{E}^T \mathbf{R}^{-1} [\mathbf{E}x_{k+1} - y_{k+1}] \right) \\ &\quad + \mathbf{E}^T \mathbf{R}^{-1} [\mathbf{E}x_k - y_k]\end{aligned}$$

- The adjoint model \mathbf{L}^T propagates μ_k (the sensitivity of J with respect to all earlier states x_k) backward in time to x_0 ;
- Each model–data misfit (i.e. innovation vector $\mathbf{E}x_k - y_k$) is a *source* of sensitivity;
- The gradient of J with respect to x_0 takes into account (and weighs) the size of *all* misfit terms, *all* (inverse) error covariances, and *all* (linearized) model dynamics.

The ocean circulation inverse problem

$$\begin{aligned}\mu_0 &= \frac{\partial J}{\partial x_0} = \sum_{1 \leq k \leq N} \frac{\partial x_k}{\partial x_0} \left(\frac{\partial J}{\partial x_k} \right) \\ &= \frac{\partial x_1}{\partial x_0} \left(\frac{\partial J}{\partial x_1} \right) + \frac{\partial x_1}{\partial x_0} \frac{\partial x_2}{\partial x_1} \left(\frac{\partial J}{\partial x_2} \right) \\ &\quad + \dots + \frac{\partial x_1}{\partial x_0} \dots \frac{\partial x_N}{\partial x_{N-1}} \left(\frac{\partial J}{\partial x_N} \right) \\ &= \mathbf{L}^T \frac{\partial J}{\partial x_1} + \mathbf{L}^T \mathbf{L}^T \frac{\partial J}{\partial x_2} + \dots + \mathbf{L}^T \dots \mathbf{L}^T \frac{\partial J}{\partial x_N}\end{aligned}$$

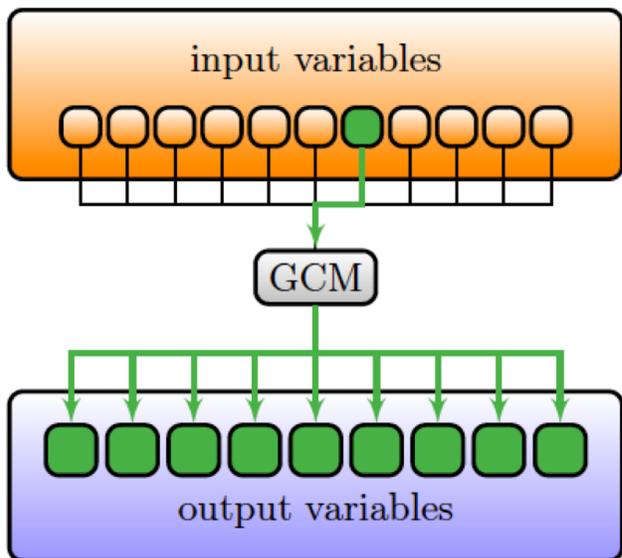
\mathbf{L}^T : is the **adjoint model** (and \mathbf{L} is the **tangent linear model**)

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

The ocean circulation inverse problem

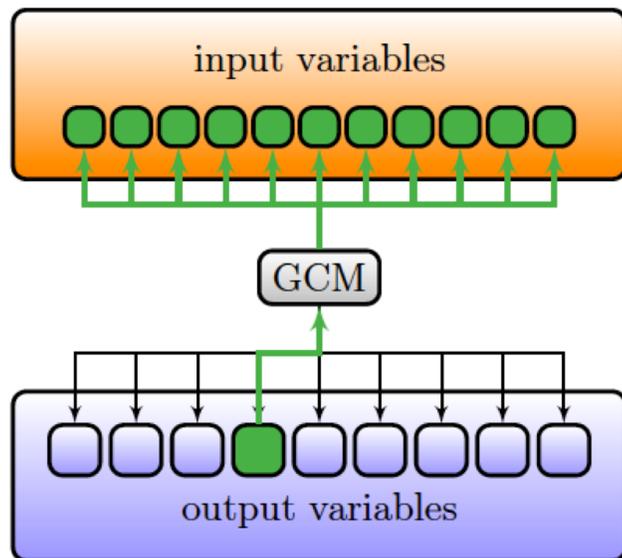
Courtesy
Nora Loose
(Oden Institute)

(a) Perturbation experiment



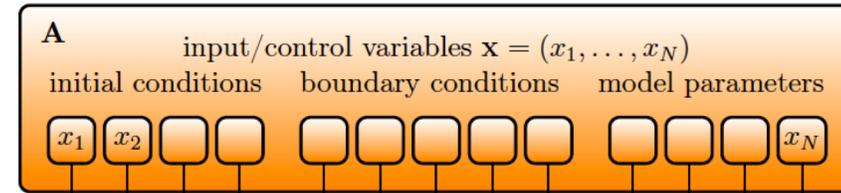
tangent linear model
 L

(b) Adjoint model

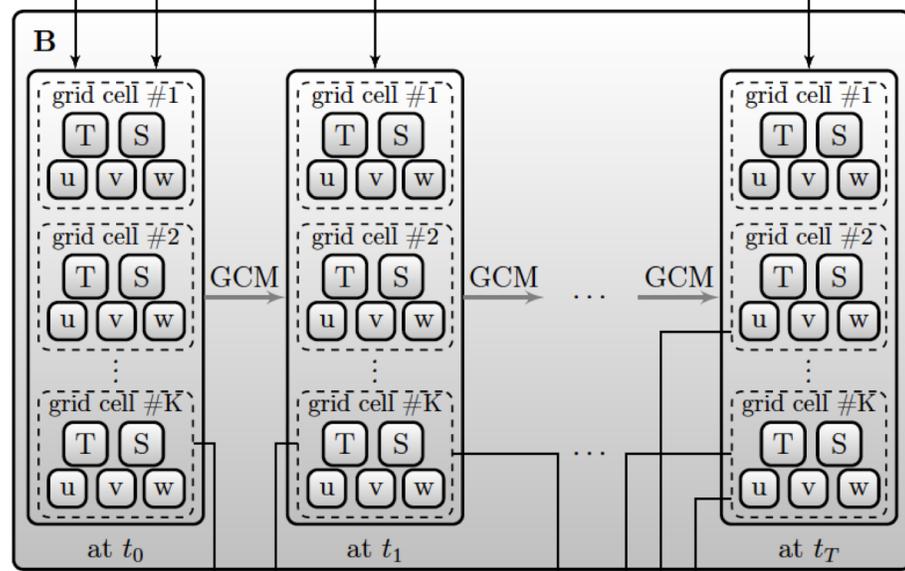


adjoint model
 L^T

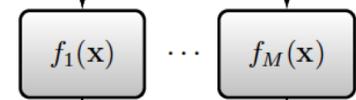
input



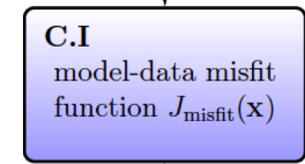
simulated ocean state



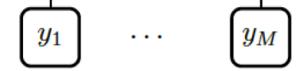
simulated observations



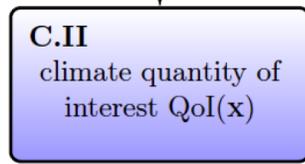
output



observations



(I) State estimation



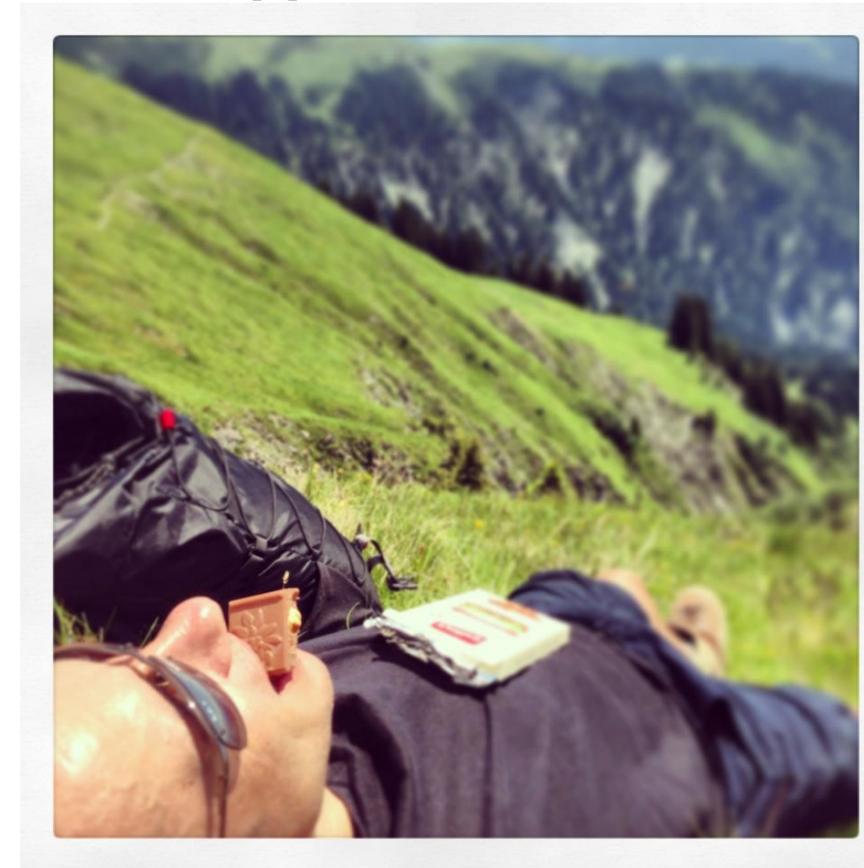
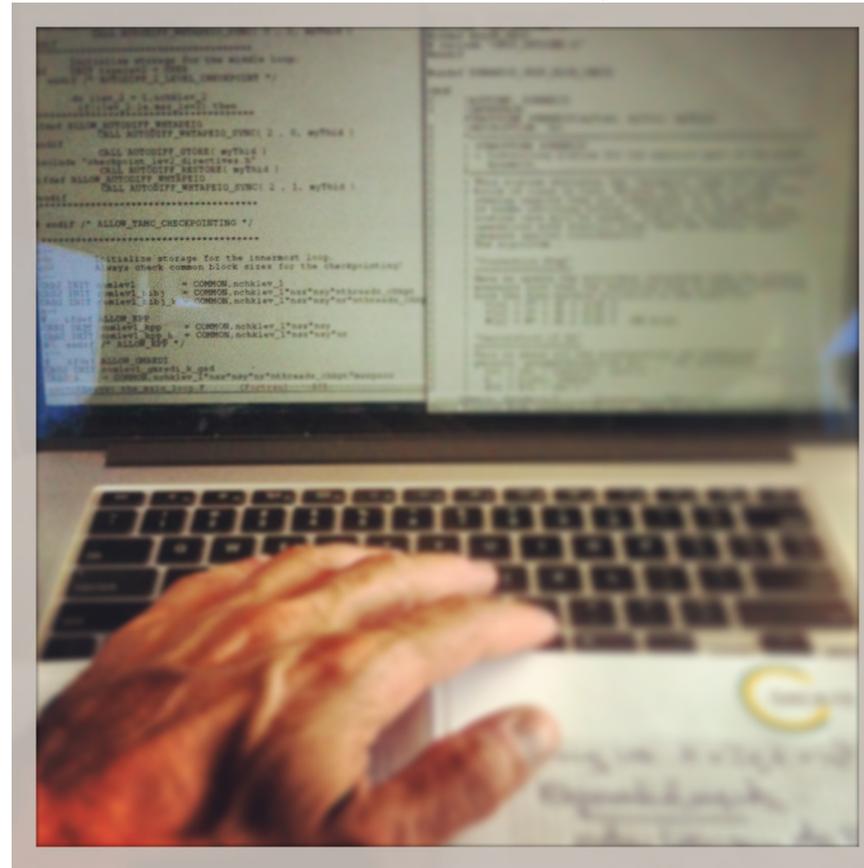
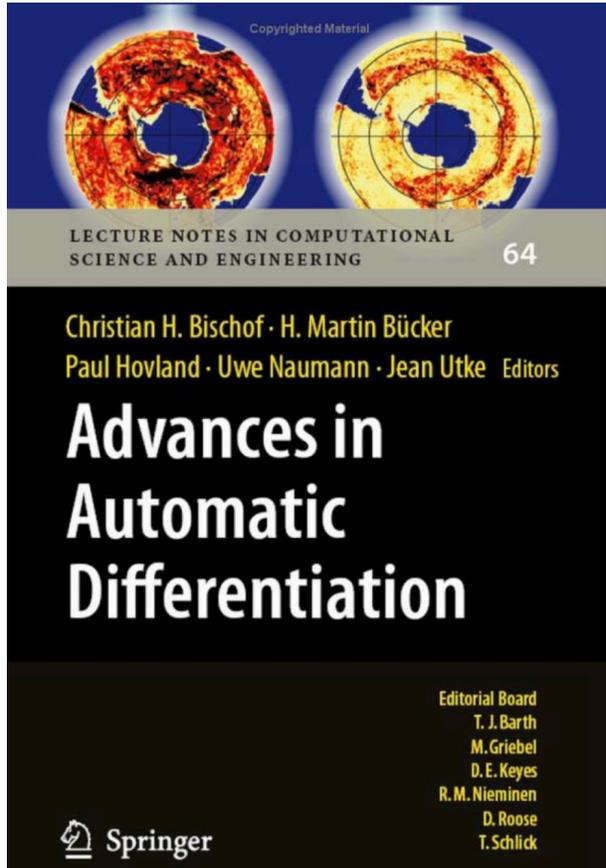
(II) Sensitivity analysis

Some of the challenges:

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

hand-written adjoint

application of AD



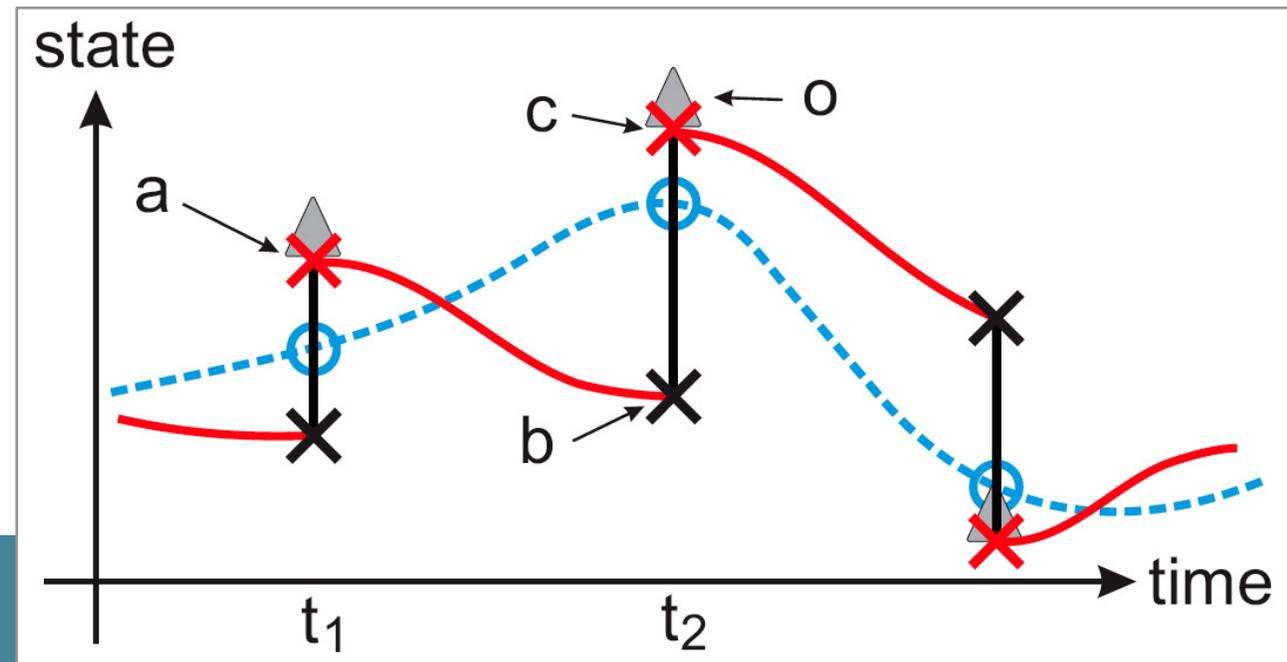
Giering & Kaminski (1998); Marotzke et al. (1999); Heimbach et al. (2005); Utke et al. (2007); Griewank & Walther (2008)

Some of the challenges:

Why adjoints: dynamical & kinematical consistency in DA

Numerical Weather Prediction (NWP) – a filtering problem

- Relatively abundant data sampling of the 3-dim. atmosphere
- NWP targets optimal forecasting
 - find initial conditions which produce best possible forecast;
 - *dynamical consistency or property conservation NOT required*



Some of the challenges:

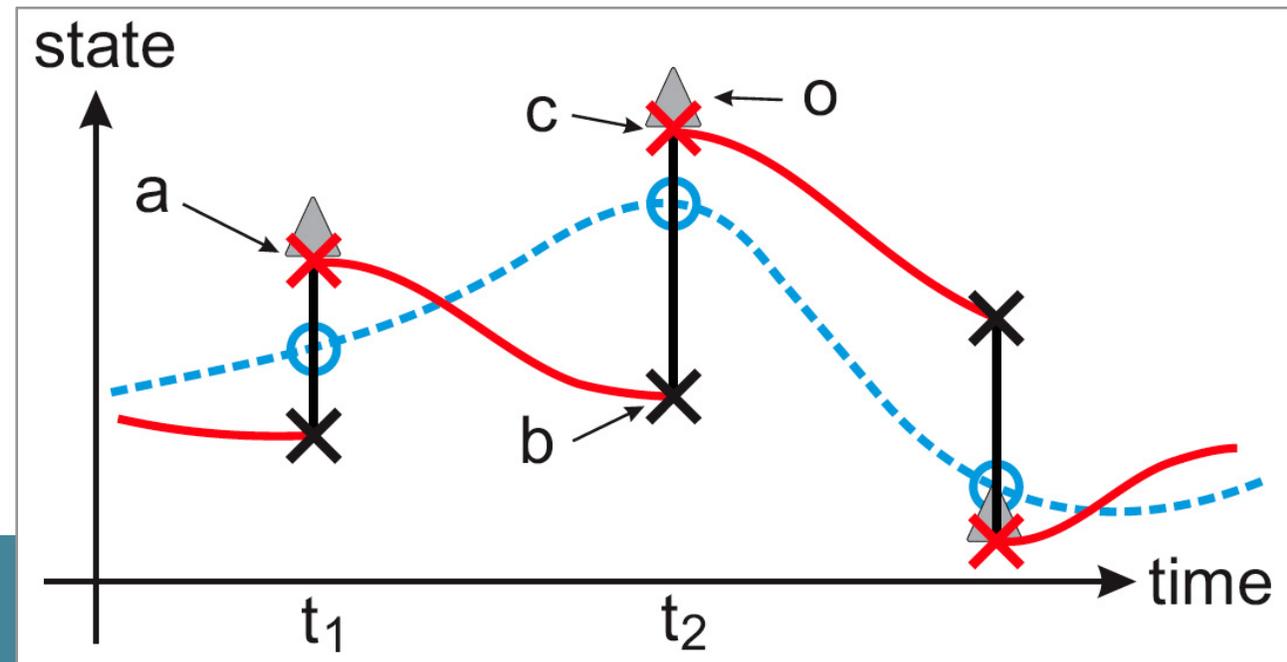
Why adjoints: dynamical & kinematical consistency in DA

Numerical Weather Prediction (NWP) – a filtering problem

- Relatively abundant data sampling of the 3-dim. atmosphere
- NWP targets optimal forecasting
 - ➔ find initial conditions which produce best possible forecast;
 - ➔ *dynamical consistency or property conservation NOT required*

Ocean state estimation/reconstruction – a smoothing problem

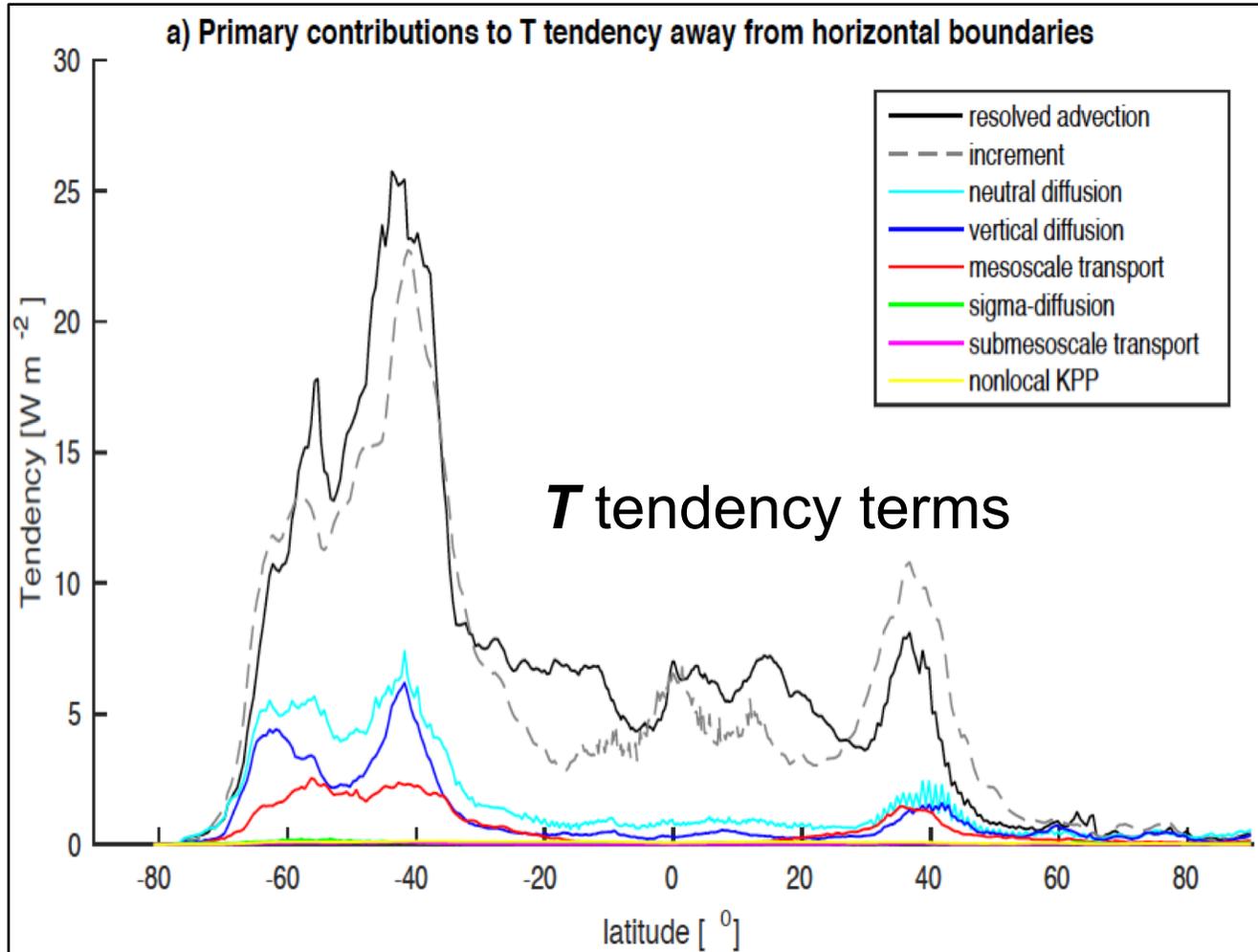
- Sparse data sampling of the 3-D. ocean
- Understanding past & present state of the ocean is a major goal all by itself
 - ➔ use observations in an optimal way
 - ➔ *dynamic consistency & property conservation ESSENTIAL* for climate



Some of the challenges:

Why adjoints: dynamical & kinematical consistency in DA

Tracer budgets in a global ocean reanalysis produced via filtering approach



Components in the tendency equation

$$dT/dt = r.h.s.$$

Unphysical analysis increments play leading role in the tracer tendencies

D. Trossman (in prep.)

Some of the challenges:

Why adjoints: dynamical & kinematical consistency in DA

Balancing the momentum, freshwater, and heat budgets



Some of the challenges:

Why adjoints: dynamical & kinematical consistency in DA

Annual mean net imbalances are **not** consistent with what we know:

- Earth Energy Imbalance ($< 1 \text{ W/m}^2$)
- Global Mean Sea Level rise ($\sim 3 \text{ mm/year}$)

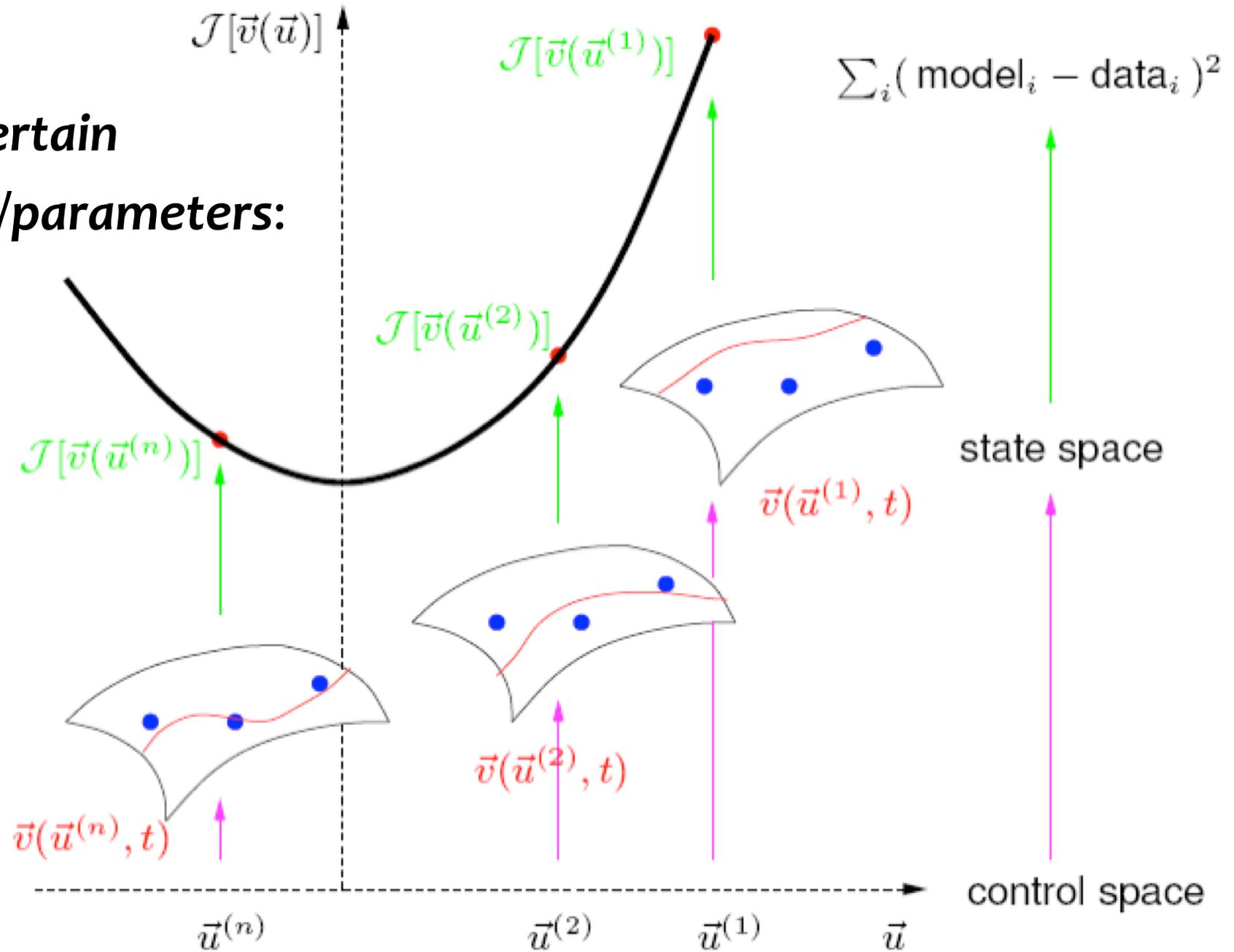
reanalysis product	net fresh water imbalance [mm/year] “+” for ocean volume increase		net heat flux imbalance [W/m ²] “+” for ocean cooling	
	ocean-only	global	ocean-only	global
NCEP/NCAR-I 1992-2010	159	62	-0.7	-2.2
NCEP/DOE-II (1992-2004)	740	-	-10	-
ERA-Interim (1992-2010)	199	53	-8.5	-6.4
JRA-25 (1992-2009)	202	70	15.3	10.1

The ocean circulation inverse problem:

The control space

*Joint inversion for uncertain
input/control variables/parameters:*

What are they?



The ocean circulation inverse problem:

The control space

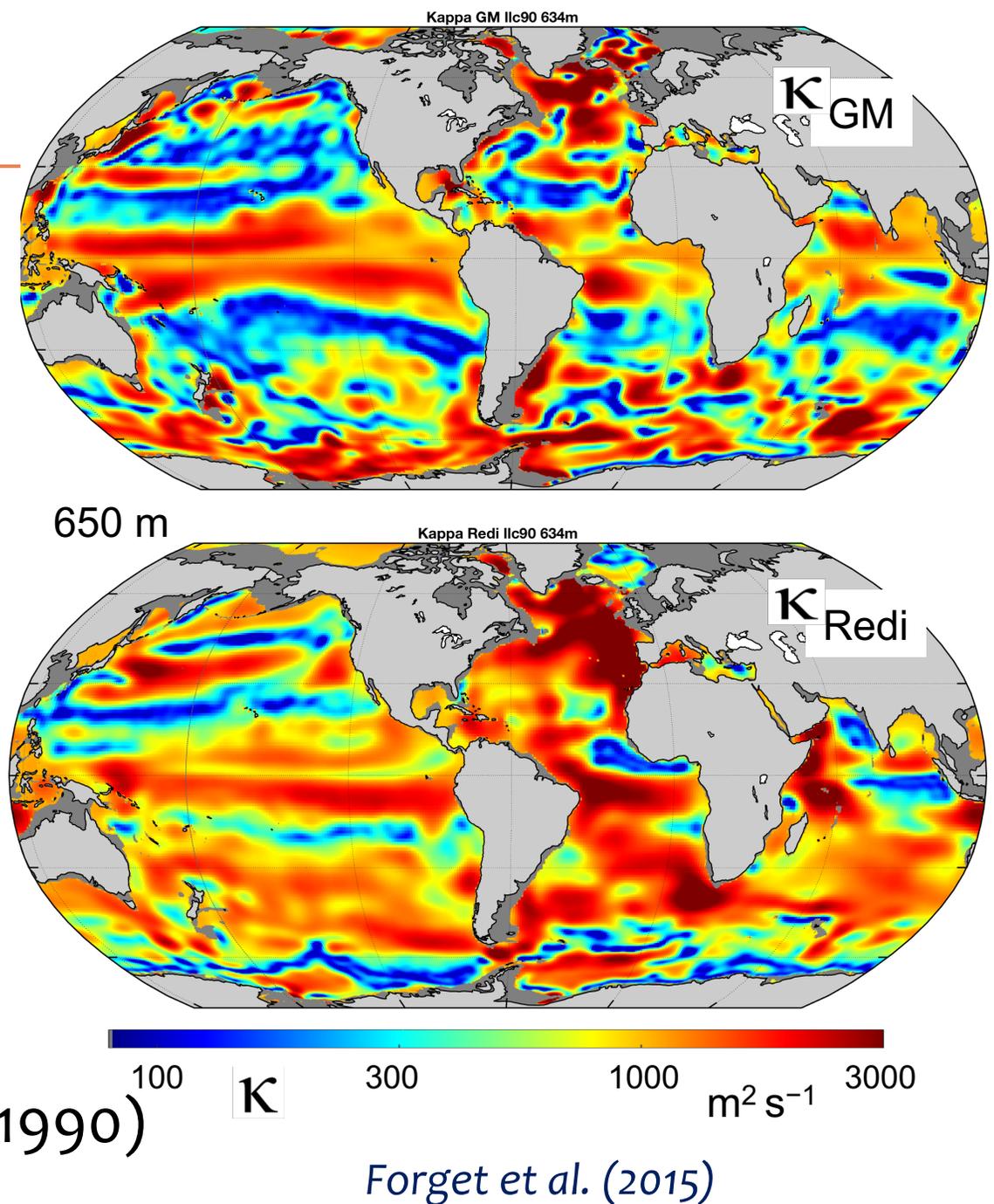
***Joint inversion for uncertain
input/control variables/parameters:***

- 3-D initial conditions (T, S, U, V)
- 2+1-D time-varying atmospheric state
(boundary conditions)

The ocean circulation inverse problem: The control space

Joint inversion for uncertain input/control variables/parameters:

- 3-D initial conditions (T, S, U, V)
- 2+1-D time-varying atmospheric state (boundary conditions)
- 3-D (time-mean) mixing parameters
 - vertical diffusivity
 - isopycnal diffusivity (Redi, 1982)
 - bolus transport (Gent-McWilliams, 1990)

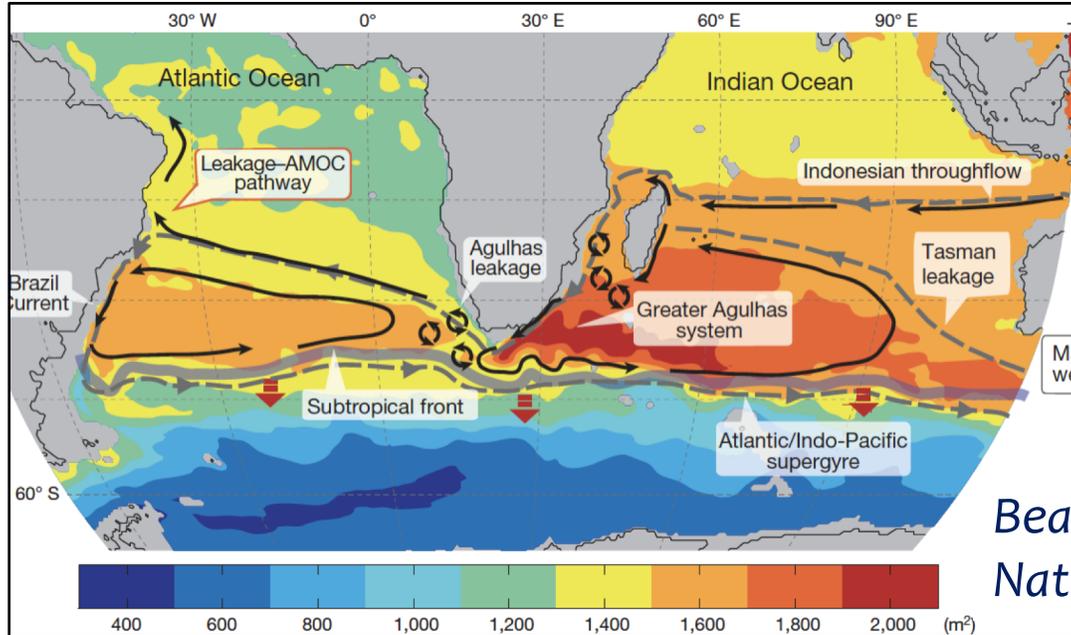


3.

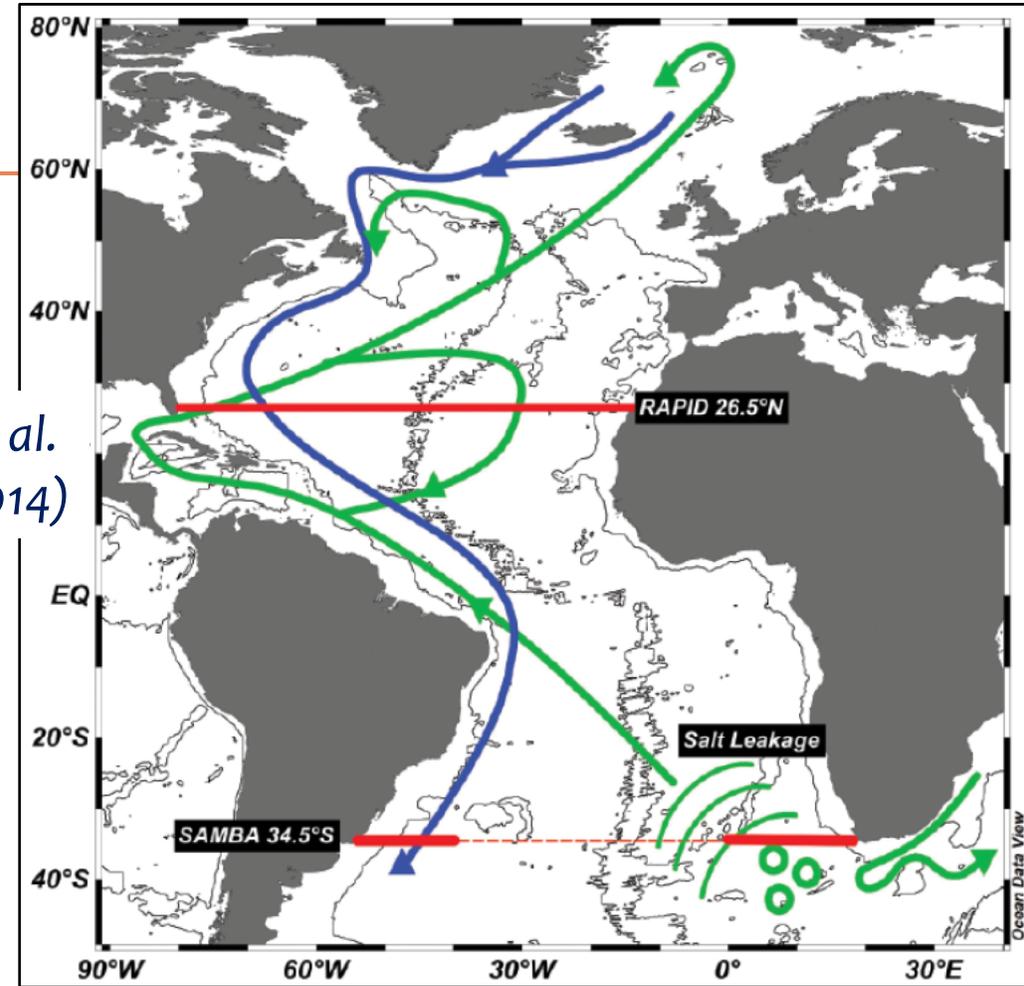
Dynamical attribution via the dual (adjoint) state

Causal / dynamical attribution: The South Atlantic Ocean Circulation

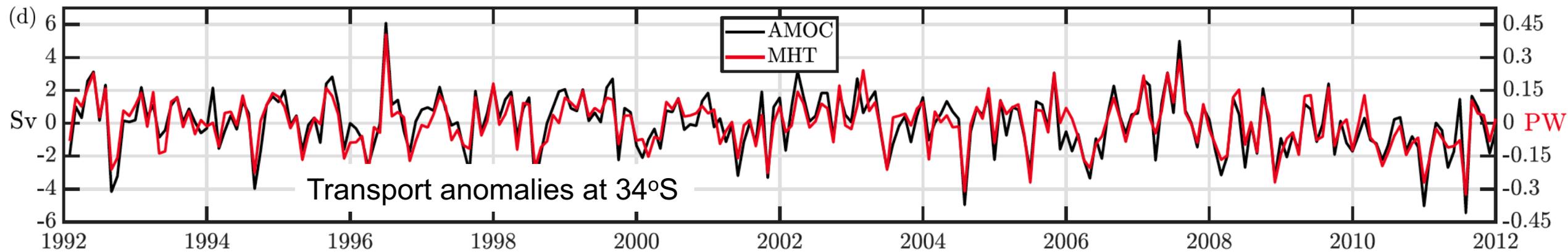
- Gateway to neighboring ocean basins
- Influences norward heat transport carried by AMOC



Beal et al.
Nature (2011)

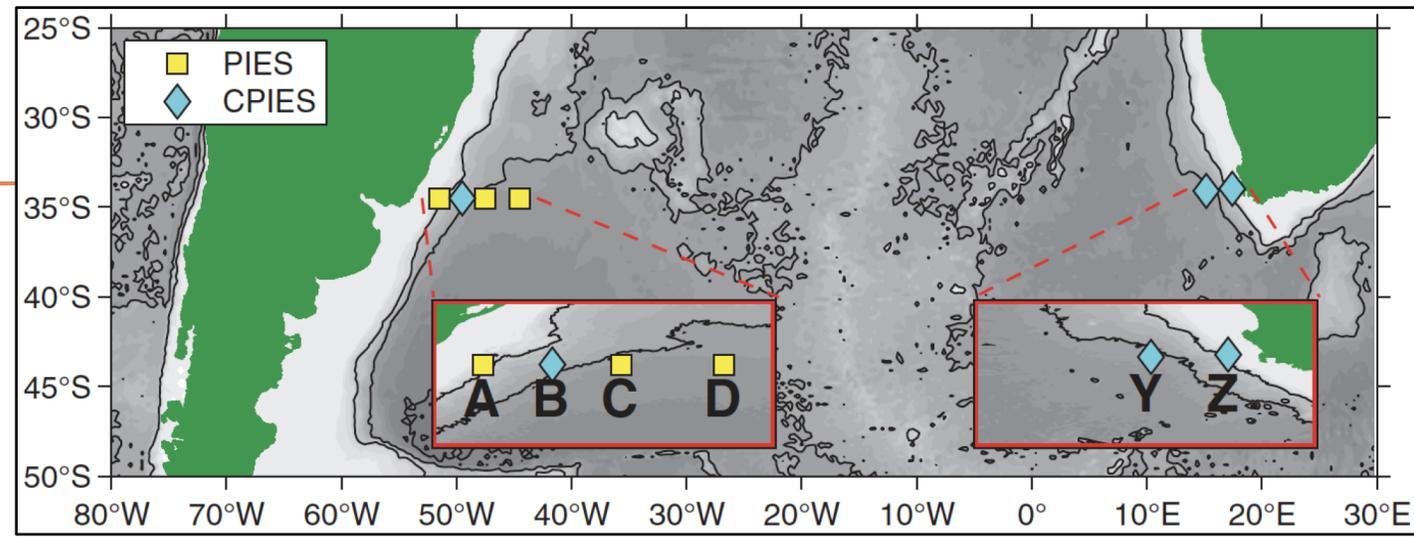


Ansorge et al.
EOS (2014)



Causal / dynamical attribution: The South Atlantic Ocean Circulation

South Atlantic Meridional Overturning Circulation (SAMOC) variability



Quantity of interest:

Smith & Heimbach, J. Clim. (2019)

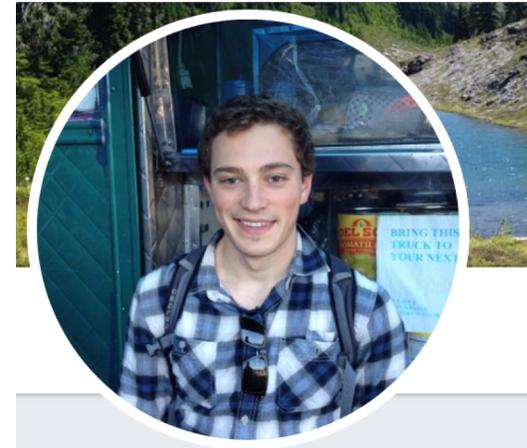
$$\delta \mathcal{J}(u(x, y, t)) \equiv \text{Monthly AMOC Anomaly @ } 34^\circ\text{S}$$

“controlled” by:

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

through (assumed) linear dynamics described by:

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



Tim Smith

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PhD candidate @utices interested in physical oceanography, inverse problems, UQ, and triathlons

📍 Austin, TX

Causal / dynamical attribution:

The South Atlantic Ocean Circulation

Now, J refers not to model vs. data misfit, but to our QoI, which is AMOC transport across 34S.

$$\begin{aligned}\mu_0 &= \frac{\partial J}{\partial x_0} = \sum_{1 \leq k \leq N} \frac{\partial x_k}{\partial x_0} \left(\frac{\partial J}{\partial x_k} \right) \\ &= \frac{\partial x_1}{\partial x_0} \left(\frac{\partial J}{\partial x_1} \right) + \frac{\partial x_1}{\partial x_0} \frac{\partial x_2}{\partial x_1} \left(\frac{\partial J}{\partial x_2} \right) \\ &\quad + \dots + \frac{\partial x_1}{\partial x_0} \dots \frac{\partial x_N}{\partial x_{N-1}} \left(\frac{\partial J}{\partial x_N} \right) \\ &= \mathbf{L}^T \frac{\partial J}{\partial x_1} + \mathbf{L}^T \mathbf{L}^T \frac{\partial J}{\partial x_2} + \dots + \mathbf{L}^T \dots \mathbf{L}^T \frac{\partial J}{\partial x_N}\end{aligned}$$

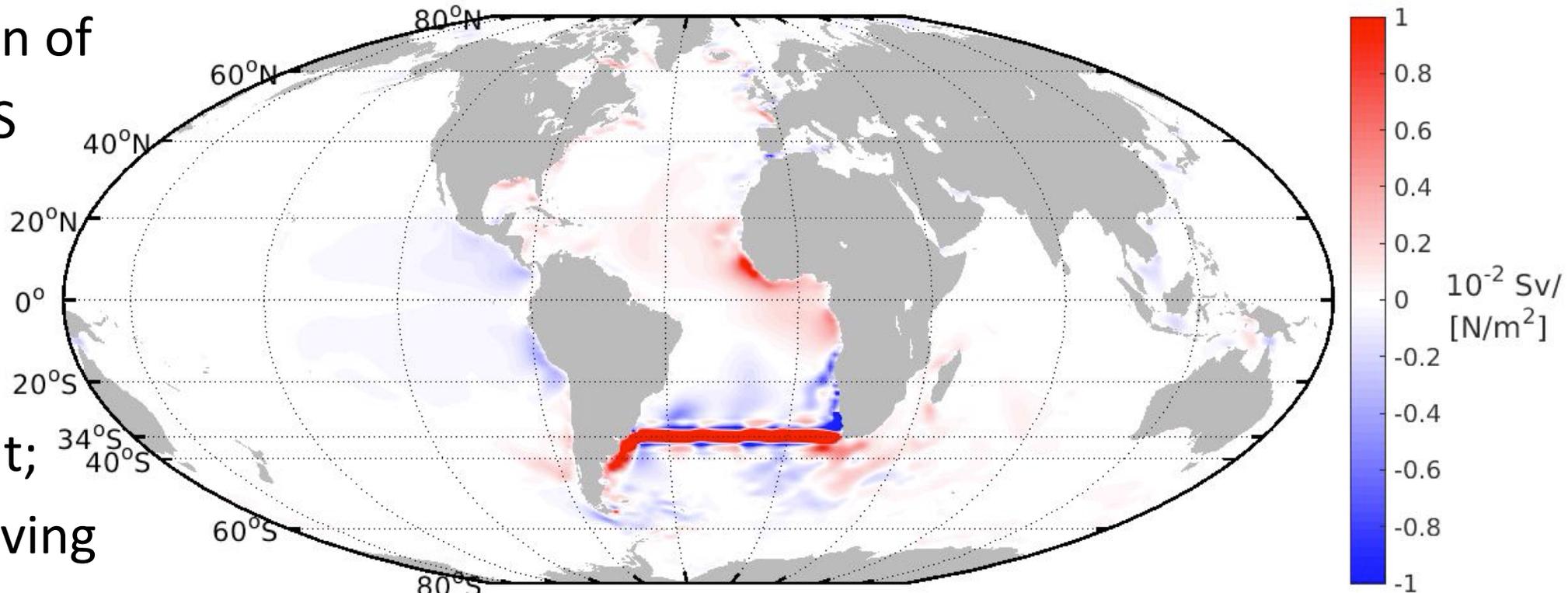
\mathbf{L}^T : is the **adjoint model** (and \mathbf{L} is the **tangent linear model**)

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

Causal / dynamical attribution:

The South Atlantic Ocean Circulation

- Use of the availability of the *dual* ocean state (i.e., the time-evolving adjoint state) for scientific analysis of sensitivity propagation.
- Reconstruction of AMOC at 33°S from forcing anomalies via the adjoint;
- The time-evolving Lagrange multipliers = dual state, has physical meaning



$$\frac{dJ}{d\tau_x}$$

$t = t_f - 0$ Days

Smith & Heimbach, J. Clim. (2019)

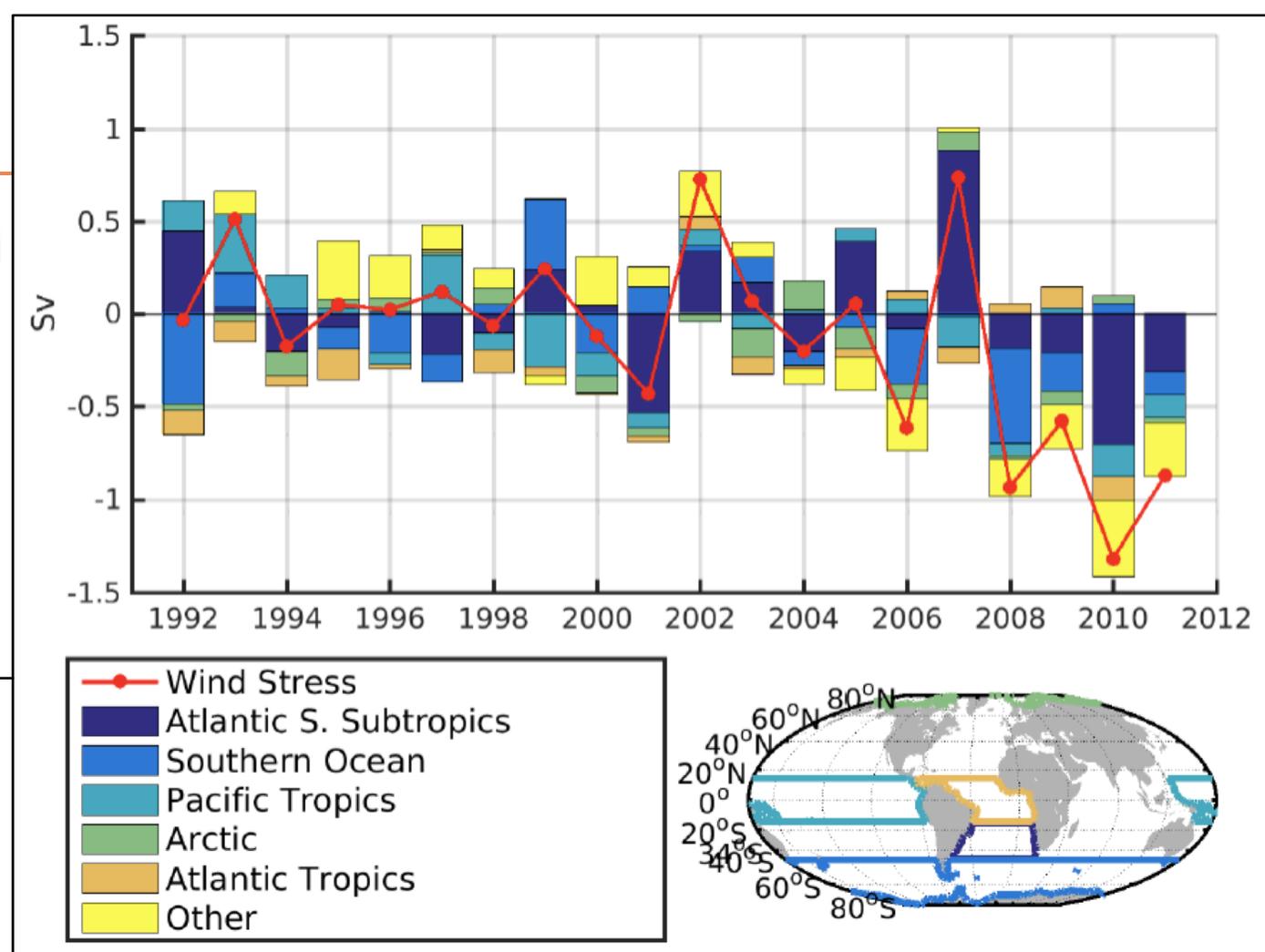
Causal / dynamical attribution: The South Atlantic Ocean Circulation

Dynamic attribution of interannual SAMOC variability due to wind stress perturbations

Smith & Heimbach, J. Clim. (2019)

$$\delta \mathcal{J}(t) = \sum_k^{N_{atm}} \delta \mathcal{J}_k(t)$$

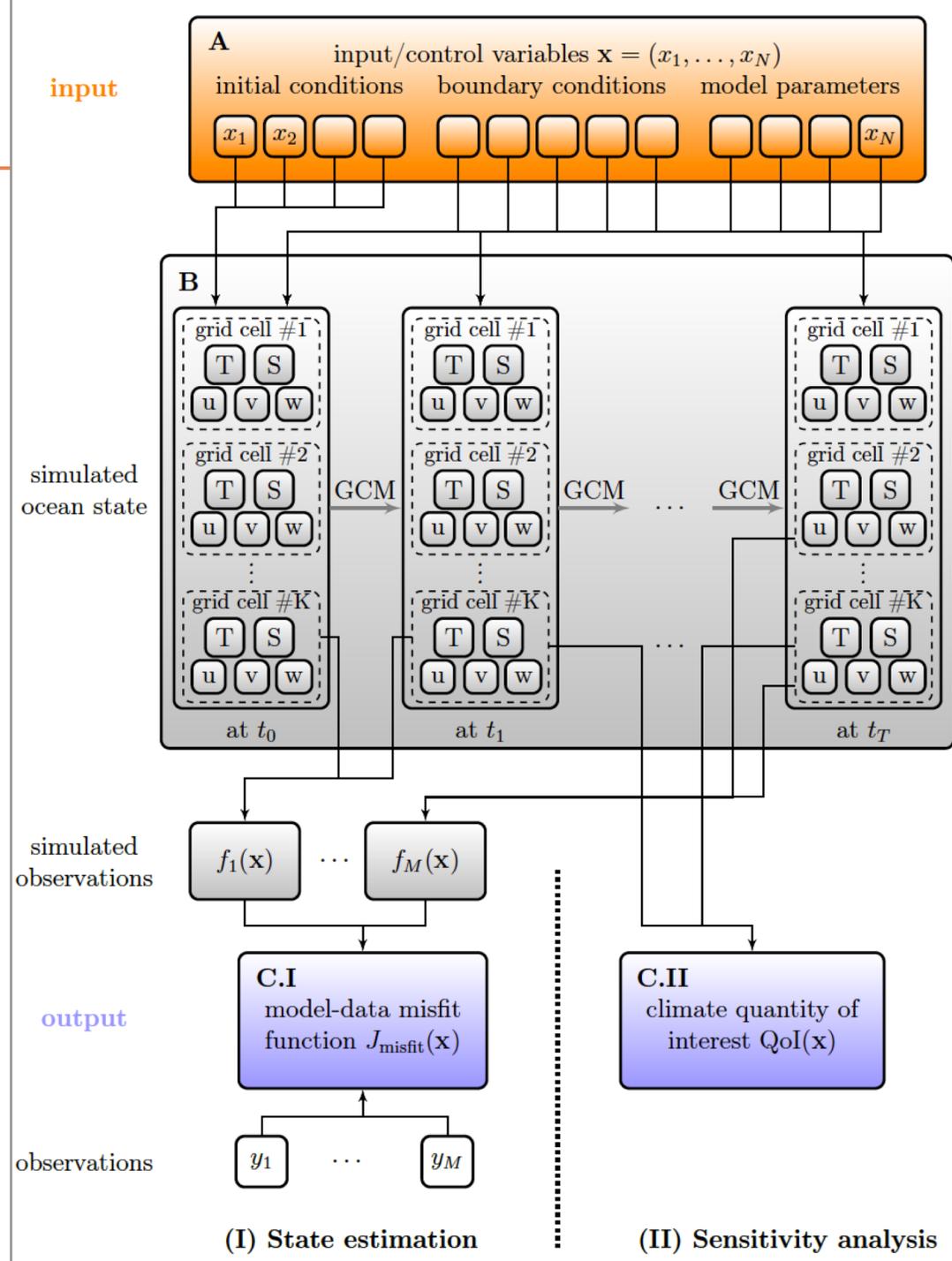
$$= \sum_k^{N_{atm}} \int_{t_0}^t \int_x \int_y \frac{\partial \mathcal{J}}{\partial u_k}(x, y, \tau - t_f) \delta u_k(x, y, \tau) dx dy d\tau$$



4.

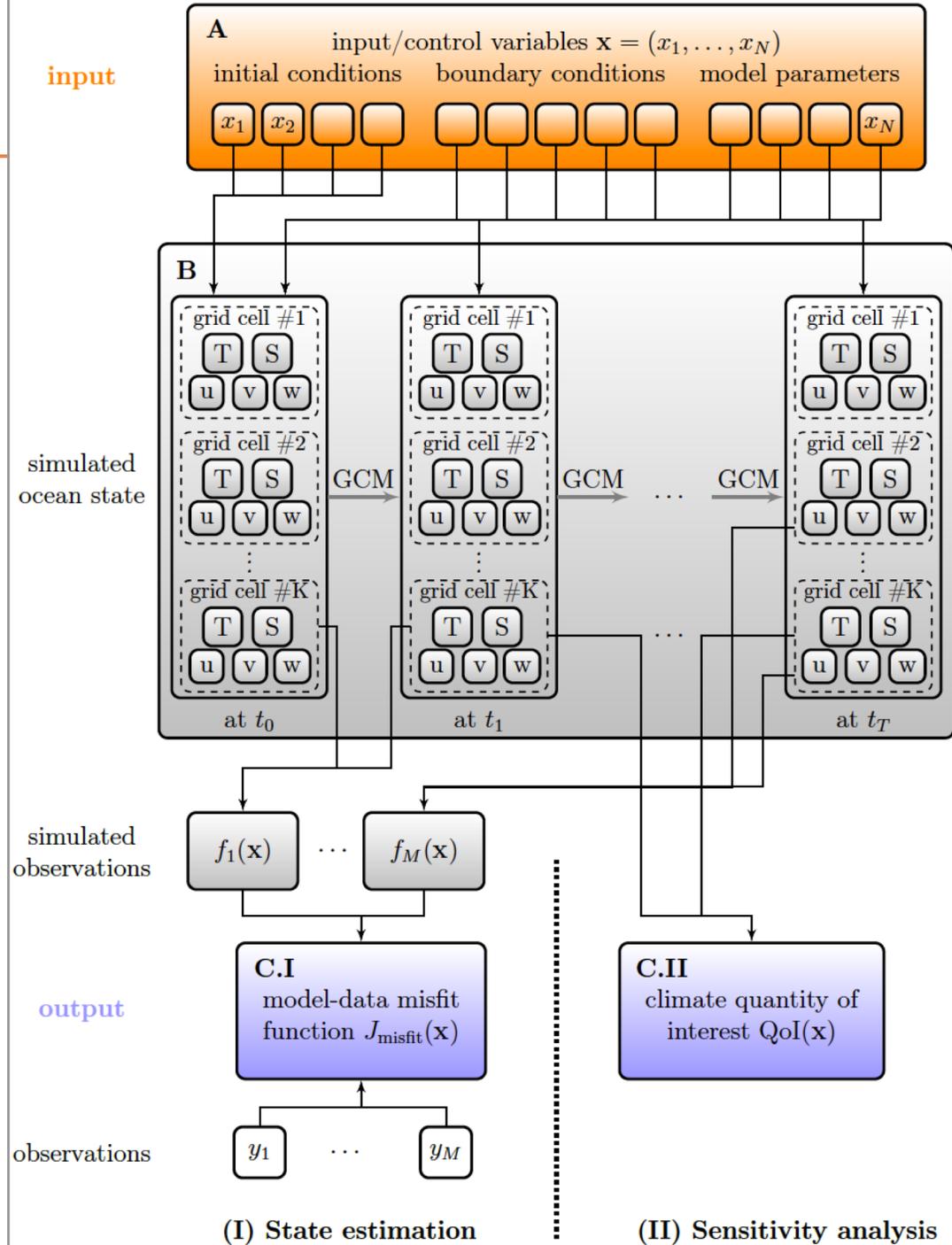
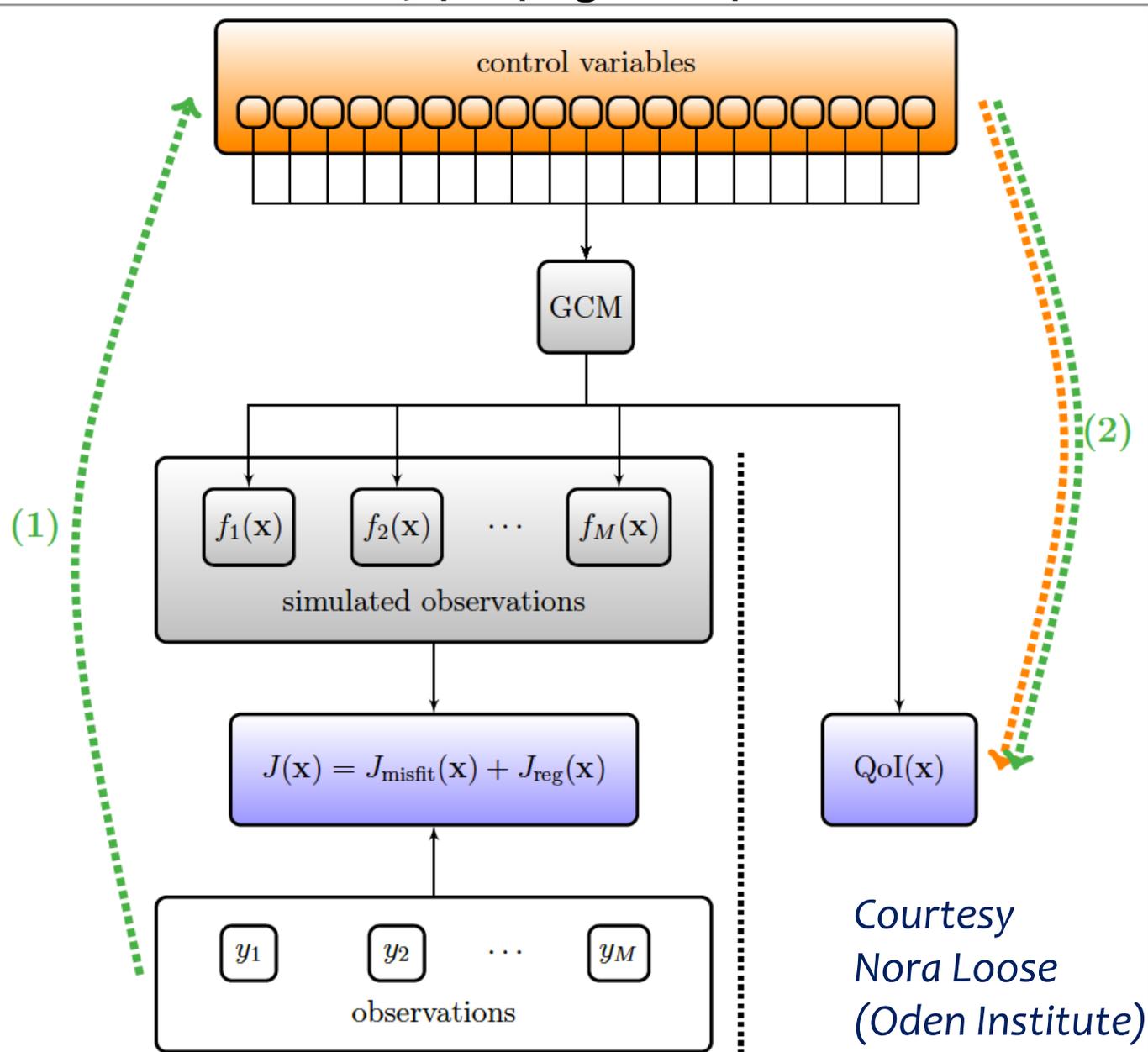
Uncertainty Quantification & Optimal Observing System Design

Recall: The inverse problem



Courtesy
 Nora Loose
 (Oden Institute)

Now: The uncertainty propagation problem



Bayesian UQ in large-scale (linear) inverse problems based on (low-rank) Hessians

$$\pi_{prior}(\mathbf{x}) \sim \exp \left[-\frac{1}{2} (\mathbf{x} - \bar{\mathbf{x}})^T \mathbf{B}^{-1} (\mathbf{x} - \bar{\mathbf{x}}) \right]$$
$$\pi_{noise}(\mathbf{e}) \sim \exp \left[-\frac{1}{2} (\mathbf{e} - \bar{\mathbf{e}})^T \mathbf{R}^{-1} (\mathbf{e} - \bar{\mathbf{e}}) \right]$$

for linear model and Gaussian prior, leads to posterior PDF:

$$\pi_{post}(\mathbf{x}) \sim \exp \left[-\frac{1}{2} \|\mathbf{x} - \bar{\mathbf{x}}\|_{\mathbf{B}}^2 - \frac{1}{2} \|\mathbf{y} - f(\mathbf{x}) - \bar{\mathbf{e}}\|_{\mathbf{R}}^2 \right]$$

with model operator $f(x) = \mathcal{L}(x)$, $\bar{\mathbf{x}} = x^b$

B: prior error covariance

R: observation & model error covariance

Bayesian UQ in large-scale (linear) inverse problems based on (low-rank) Hessians

- Hessian and prior-preconditioned Hessian of the data misfit:

$$\begin{aligned}H_{misfit} &= L^T R^{-1} L \\ \tilde{H}_{misfit} &= B^{1/2} H_{misfit} B^{1/2} = B^{1/2} L^T R^{-1} L B^{1/2} \\ &= V \Lambda V^T\end{aligned}$$

- Posterior error covariance:

$$\begin{aligned}P &= \left(L^T R^{-1} L + B^{-1} \right)^{-1} \\ &= B^{1/2} \left(B^{1/2} L^T R^{-1} L B^{1/2} + I \right)^{-1} B^{1/2} \\ &= B^{1/2} \left(V \Lambda V^T + I \right)^{-1} B^{1/2}\end{aligned}$$

Bayesian UQ in large-scale (linear) inverse problems based on (low-rank) Hessians

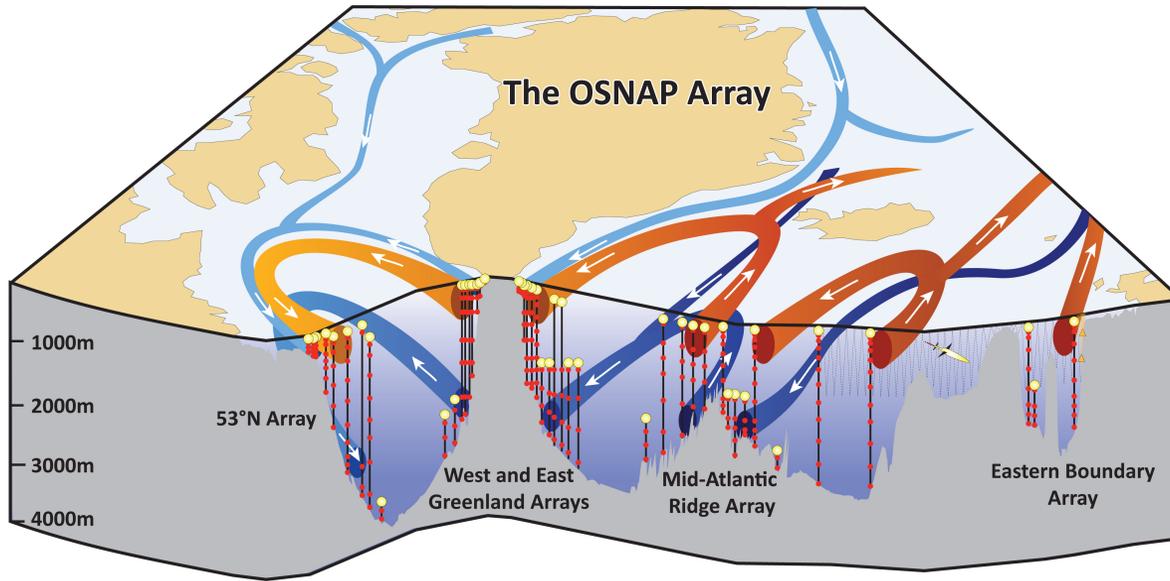
Inversion using Sherman-Morrison-Woodbury relation:

$$\begin{aligned} & \left(B^{1/2} L^T R^{-1} L B^{1/2} + I \right)^{-1} \\ &= I - V_r D_r V_r^T + \mathcal{O} \left(\sum_{i=r+1}^n \frac{\lambda_i}{\lambda_i + 1} \right) \end{aligned}$$

with Λ_r , V_r truncated eigenvalues & eigenvector matrix

$$\begin{aligned} P &= B^{1/2} \left(I - V_r D_r V_r^T \right) B^{1/2}, \quad D_r = \text{diag} \left(\frac{\lambda_i}{\lambda_i + 1} \right) \\ &= B^{1/2} \left\{ I - \sum_{i=1}^{N_{\text{obs}}} d_i v_i v_i^T \right\} B^{1/2}, \quad d_i = \frac{\lambda_i}{\lambda_i + 1} \end{aligned}$$

Bayesian UQ in large-scale (linear) inverse problems based on (low-rank) Hessians



Overturning in the Subpolar North Atantic Program (OSNAP)

<http://www.o-snap.org>

Lozier et al., *BAMS* (2017)

Lozier et al., *Science* (2019)



Nora Loose

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Research fellow at UT Austin & PhD student at the University of Bergen. Mathematician, physical oceanographer, climate scientist.

📍 Austin, TX

N. Loose, PhD thesis (2019)

Bayesian UQ in large-scale (linear) inverse problems based on (low-rank) Hessians

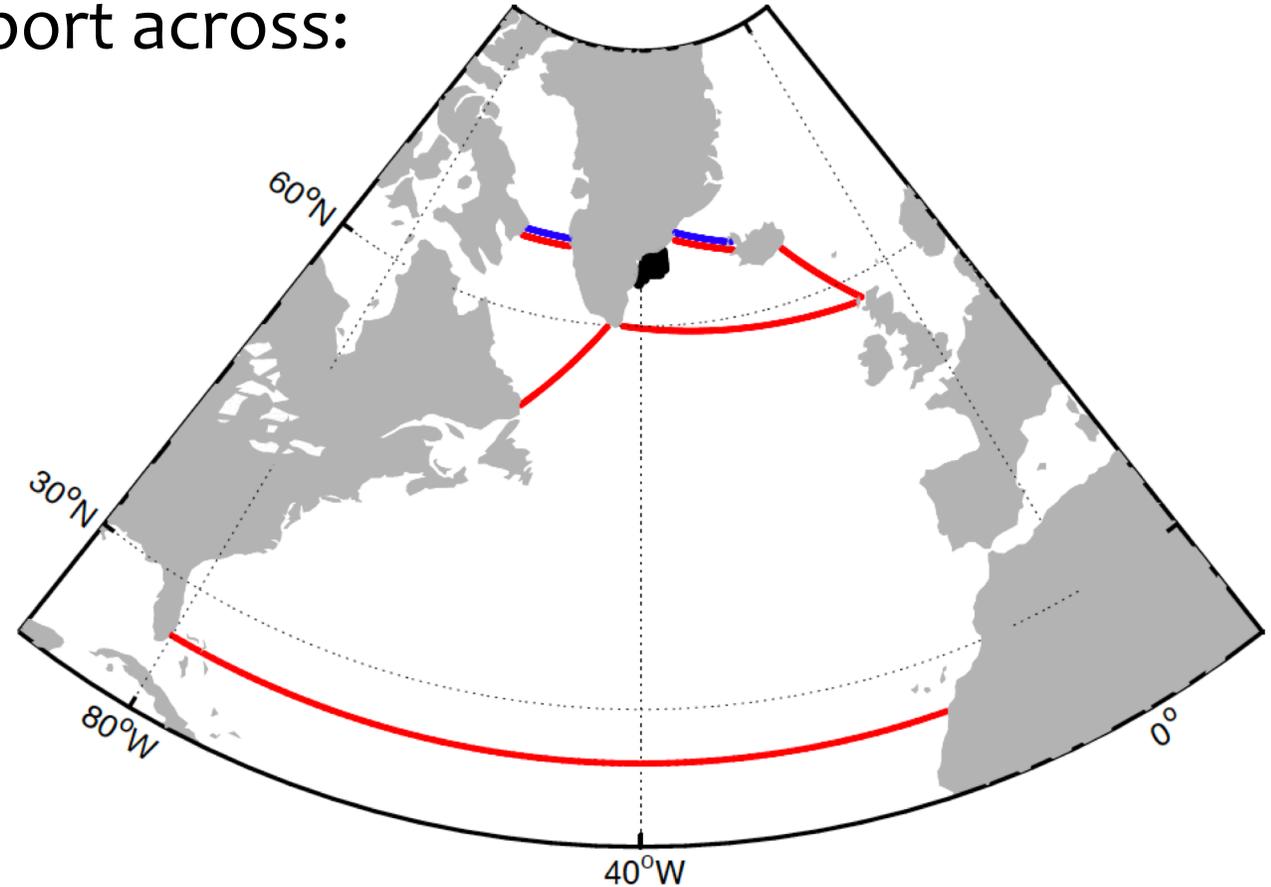
Observations: heat & volume transport across:

- Iceland-Scotland Ridge
- RAPID array (26N)
- OSNAP West
- OSNAP East
- Davis Strait

Quantity of Interest (QoI):

subsurface heat content outside of

Sermilik Fjord & Helheim Glacier (Southeast Greenland)



N. Loose, PhD thesis (2019)

How well does each observing system constrain the solution & relevant QoIs?

Prior & posterior variances of Quantity of Interest Q

$$\mu_{prior} = \left(\frac{\partial Q}{\partial x} \right)^T B \left(\frac{\partial Q}{\partial x} \right), \quad \mu_{post} = \left(\frac{\partial Q}{\partial x} \right)^T P \left(\frac{\partial Q}{\partial x} \right)$$

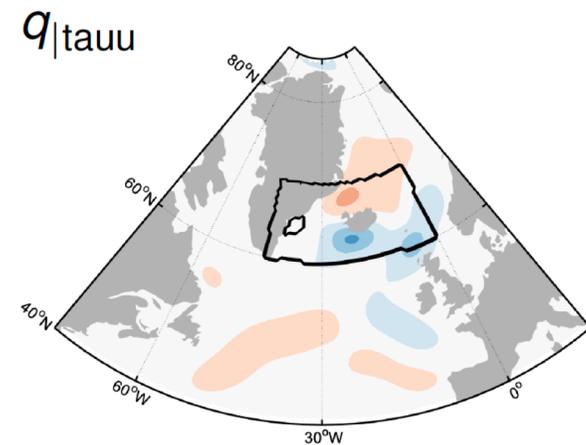
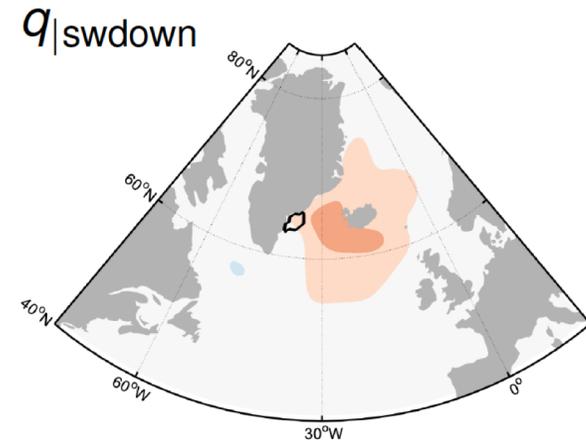
Case of only 1 observation:

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

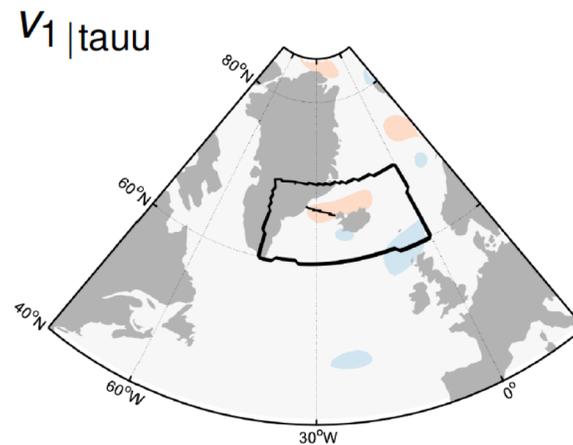
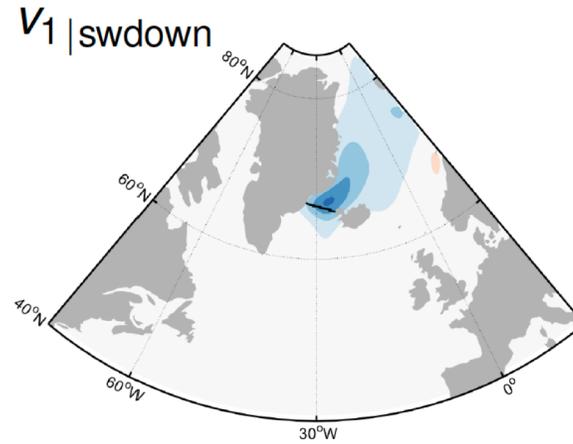
$$1 - \frac{\mu_{post}}{\mu_{prior}} = d_1 \left\langle \frac{B^{1/2} \left(\frac{\partial Q}{\partial x} \right)^T}{\|B^{1/2} \left(\frac{\partial Q}{\partial x} \right)^T\|}, \frac{B^{1/2} \left(\frac{\partial \mathcal{J}}{\partial x} \right)^T}{\|B^{1/2} \left(\frac{\partial \mathcal{J}}{\partial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

How well does each observing system constrain the solution & relevant QoIs?

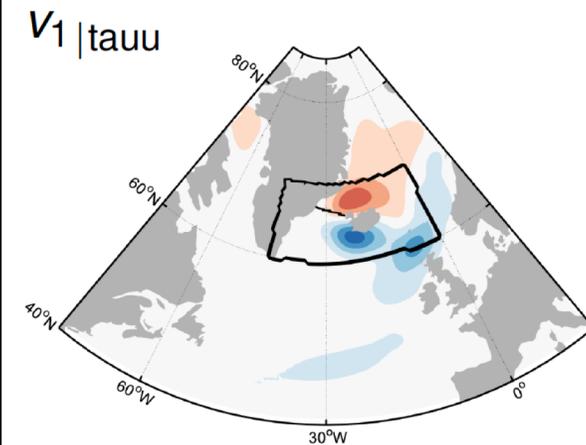
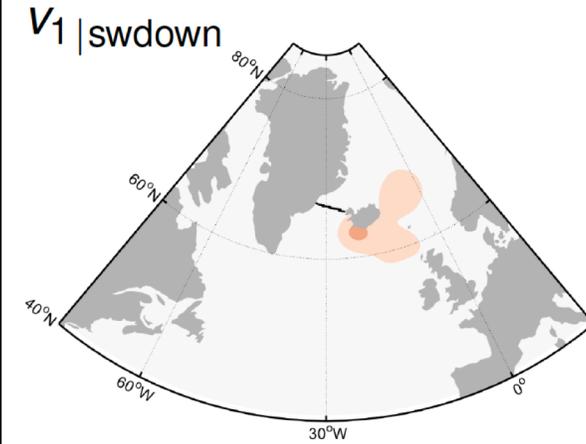
QoI = subsurface
temperature near Helheim



Obs₁ = **heat transport**
across DS



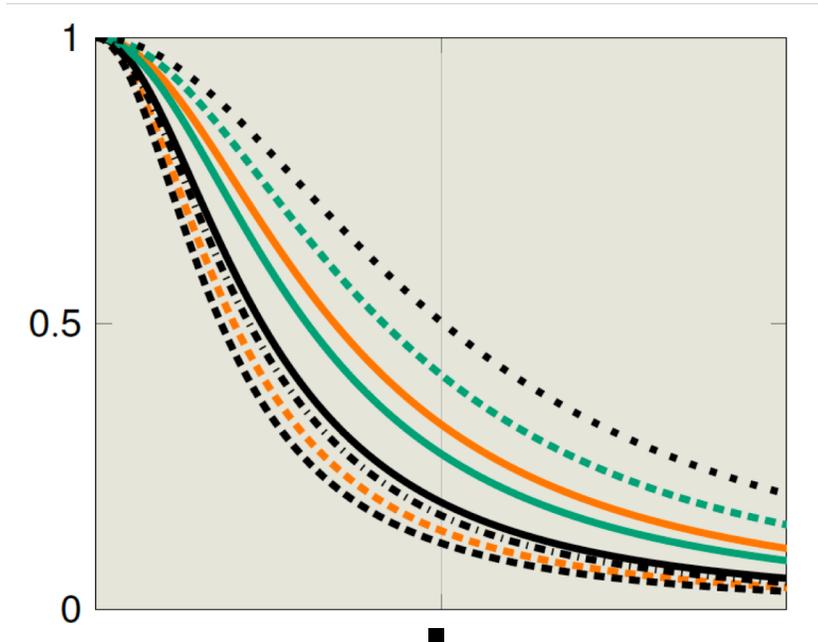
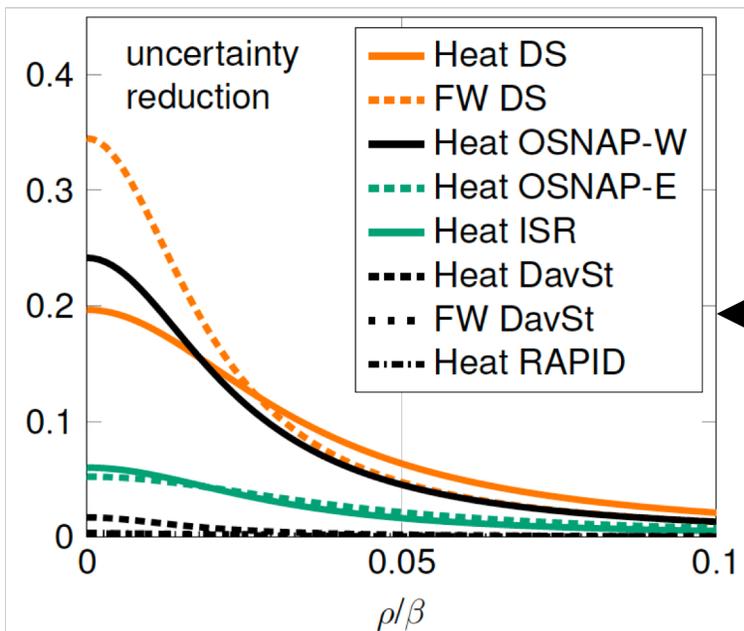
Obs₂ = **volume transport**
across DS



N. Loose, PhD thesis (2019)

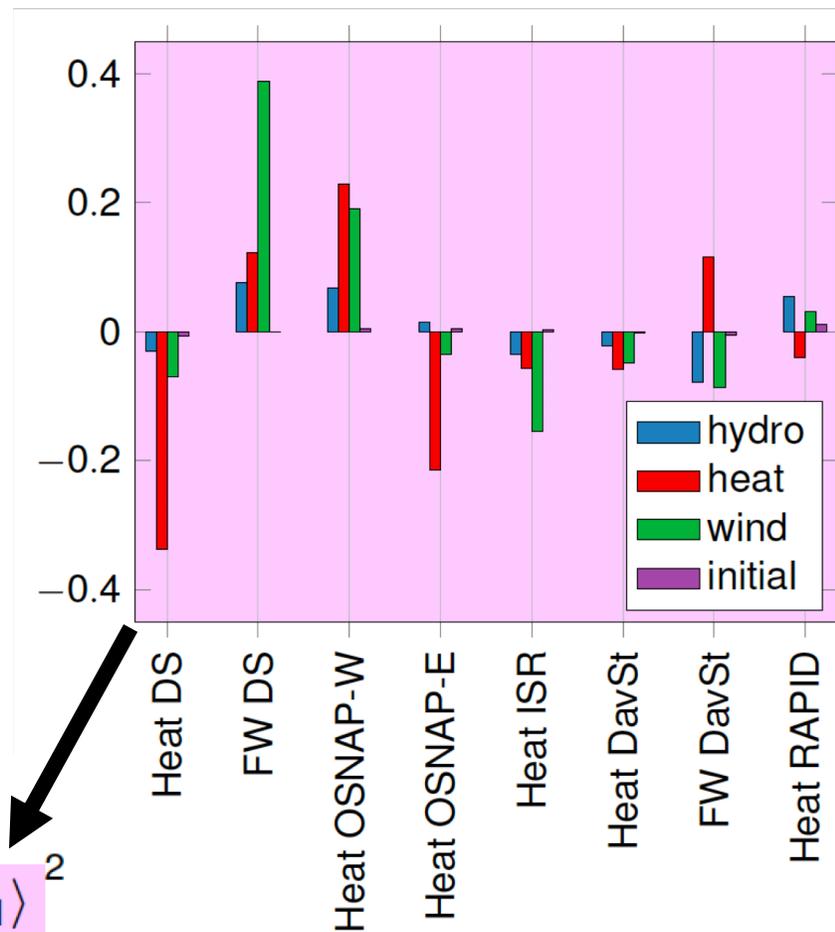
How well does each observing system constrain the solution & relevant QoIs?

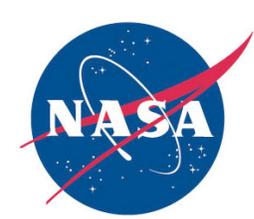
Uncertainty Reduction



$$\frac{\left\| \mathbf{B}^{1/2} \left[\frac{\partial(\text{Obs})}{\partial \mathbf{x}} \right]^T \right\|^2}{\left(\left\| \mathbf{B}^{1/2} \left[\frac{\partial(\text{Obs})}{\partial \mathbf{x}} \right]^T \right\|^2 + \frac{\rho^2}{\beta^2} \varepsilon^2 \right)}$$

$$\langle q, v_1 \rangle^2$$



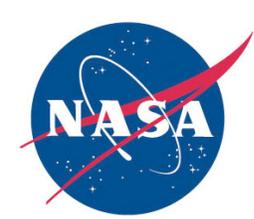


Conclusions: optimal state & parameter estimation
A unified, data-driven computational framework that enables:



1. Model calibration & state reconstruction via gradient-based optimization
 - making optimal use of available, disparate observing systems
 - dynamical & kinematical consistency of data-model synthesis
2. Causal / dynamical attribution of observed changes
 - Adjoint / dual state propagates sensitivity information
 - Dynamical attribution via convolution
3. Hessian-based uncertainty quantification
 - Prior –to– posterior –to– QoI uncertainty propagation
4. Optimal Experimental (Observing System) Design

A long-term program to bring to bear CSE tools in ocean climate modeling



Acknowledgement



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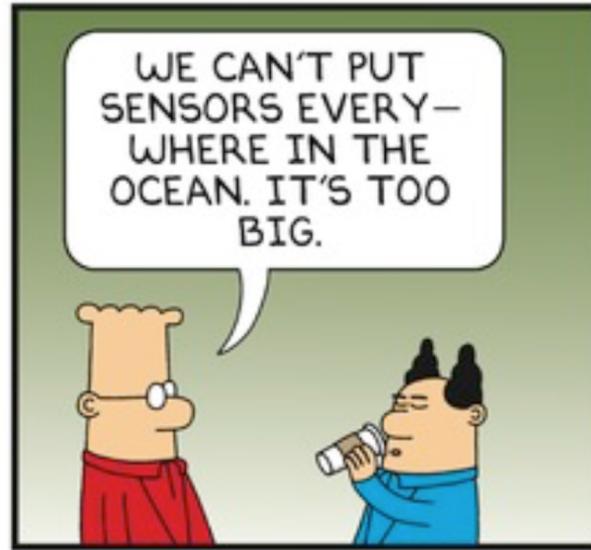
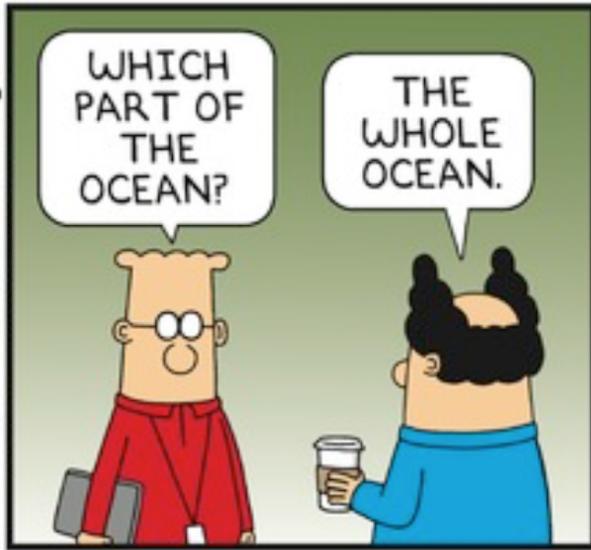
*ECCO Group
& Friends*

<http://ecco-group.org>

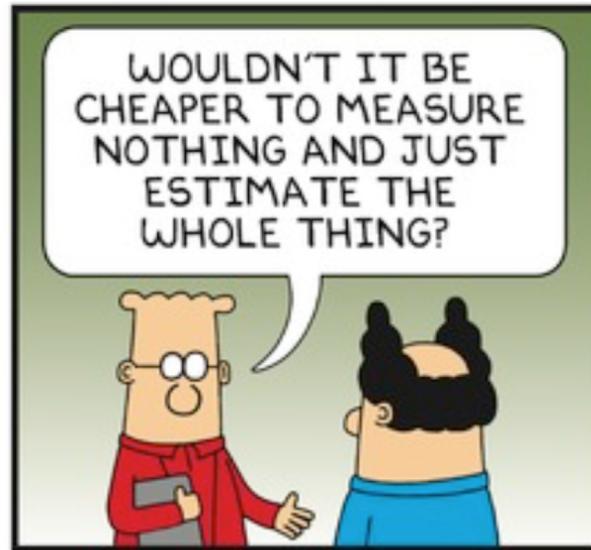
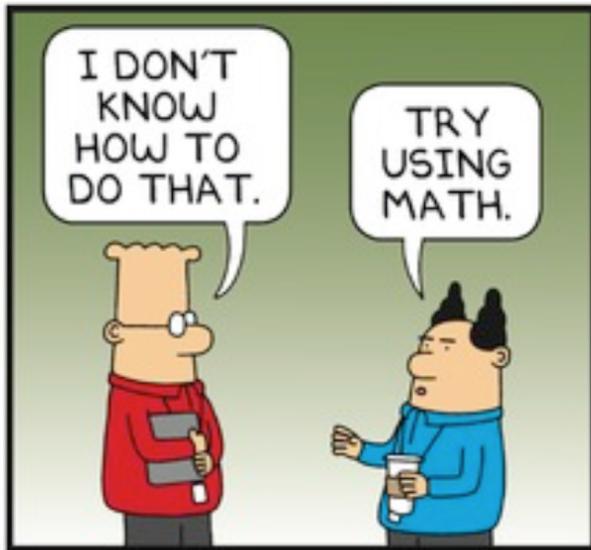
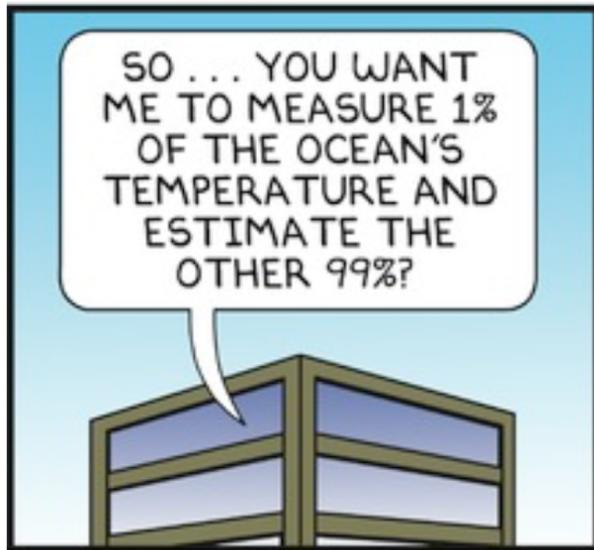




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