Uncertainty Quantification (UQ) in Global Ocean State Estimation

Alex Kalmikov and Patrick Heimbach

with Carl Wunsch

Department of Earth, Atmospheric and Planetary Sciences (EAPS)

Massachusetts Institute of Technology, Cambridge MA

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Estimating the Circulation and Climate of the Ocean

http://ecco-group.org

http://mitgcm.org

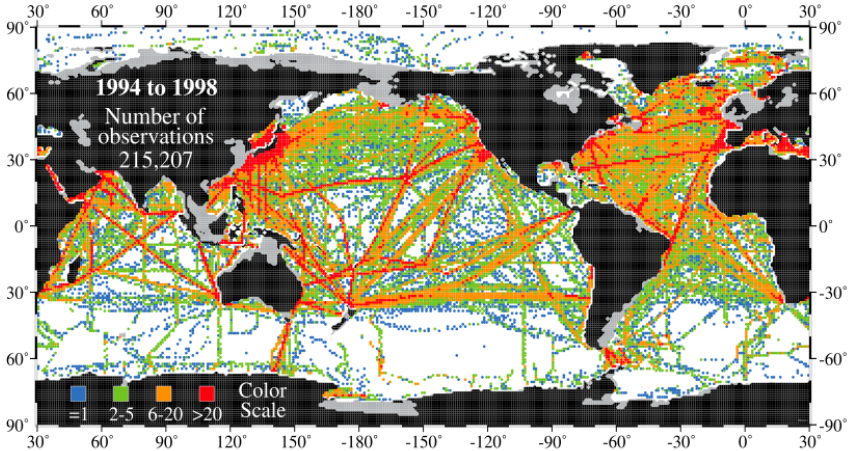
Outline

1. Global ocean state estimation for climate
   - motivation and objectives
2. Quantifying uncertainties of the state estimate and associated climate diagnostics
   - Algorithmic Differentiation (AD)
   - the Hessian method
3. Example: Volume transport through Drake Passage
   - Antarctic Circumpolar Current (ACC)
   - MITgcm in barotropic configuration
4. Results
   - inverse-to-forward UQ propagation
   - uncertainty propagation mechanisms
   - time-resolving UQ
   - posterior uncertainty reduction

Global Ocean State Estimation

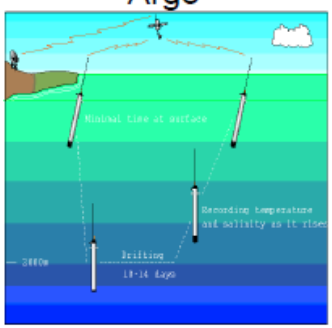
- Combination of ocean **models** with **observations**
- Dynamically and kinematically consistent reconstruction of ocean
  - fields, evolution, dynamics
- “Data assimilation”, “reanalysis”
- **Estimation** (interpolation) vs. **forecasting** (extrapolation) problem
- Sparse observations (*in space & time*), restricted (*mostly*) to upper ocean layers

In-situ observations



T/P, Jason

Argo



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

UQ framework for ocean state estimation

- Estimation problem: Data → Controls → Target

  $\mathbf{y} \rightarrow \mathbf{x} \rightarrow \mathbf{z}$

- Uncertainty problem: Data uncertainty → Controls uncertainty → Target uncertainty

  $\Delta\mathbf{y} \rightarrow \Delta\mathbf{x} \rightarrow \Delta\mathbf{z}$

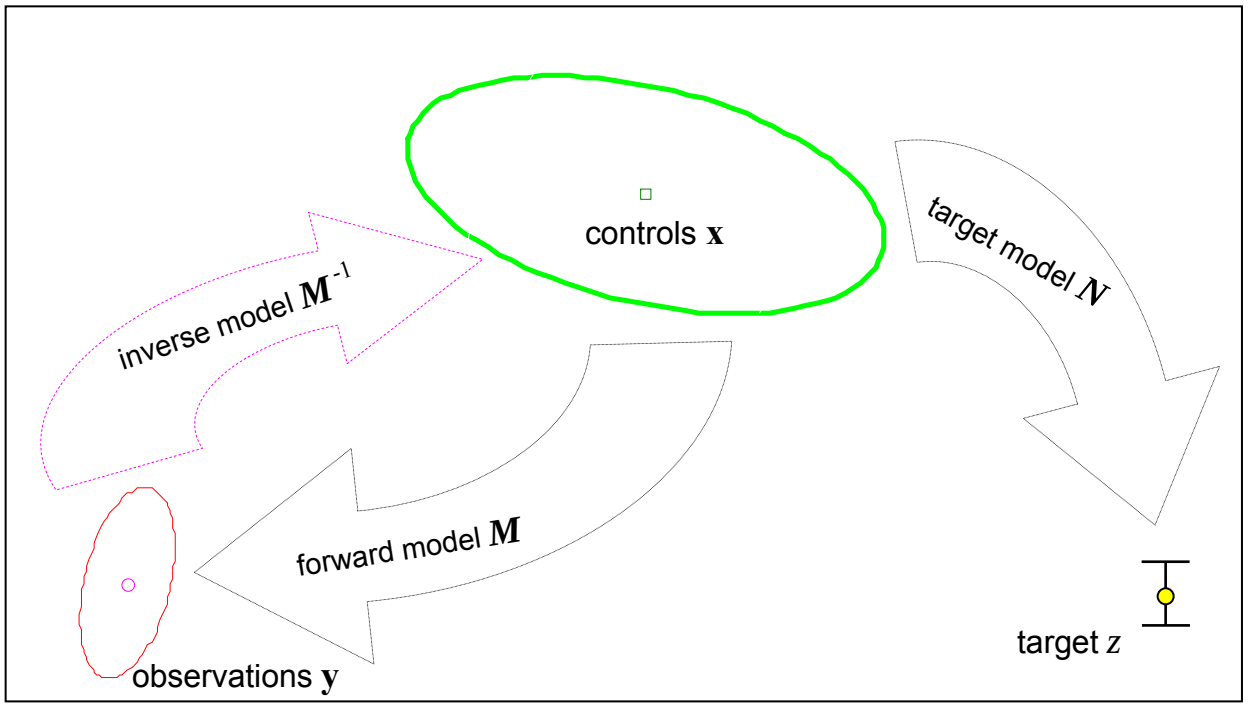
Examples: observed surface elevation

- initial surface elevation
- wind forcing

mass transport

$\mathbf{x}$ – unknowns (e.g. parameters, state, controls, model error)

- Observations (forward) model
  $\mathbf{y} = \boldsymbol{M}(\mathbf{x})$
- Inverse model
  $\mathbf{x} = \boldsymbol{M}^{-1}(\mathbf{y})$
- Target model
  $\mathbf{z} = \boldsymbol{N}(\mathbf{x}) = \boldsymbol{N}\left(\boldsymbol{M}^{-1}(\mathbf{y})\right)$



Adjoint method - estimation

- **Nonlinear Inverse Problem:** $\mathbf{y} = \boldsymbol{M}(\mathbf{x}) \rightarrow \mathbf{x} = \boldsymbol{M}^{-1}(\mathbf{y})$

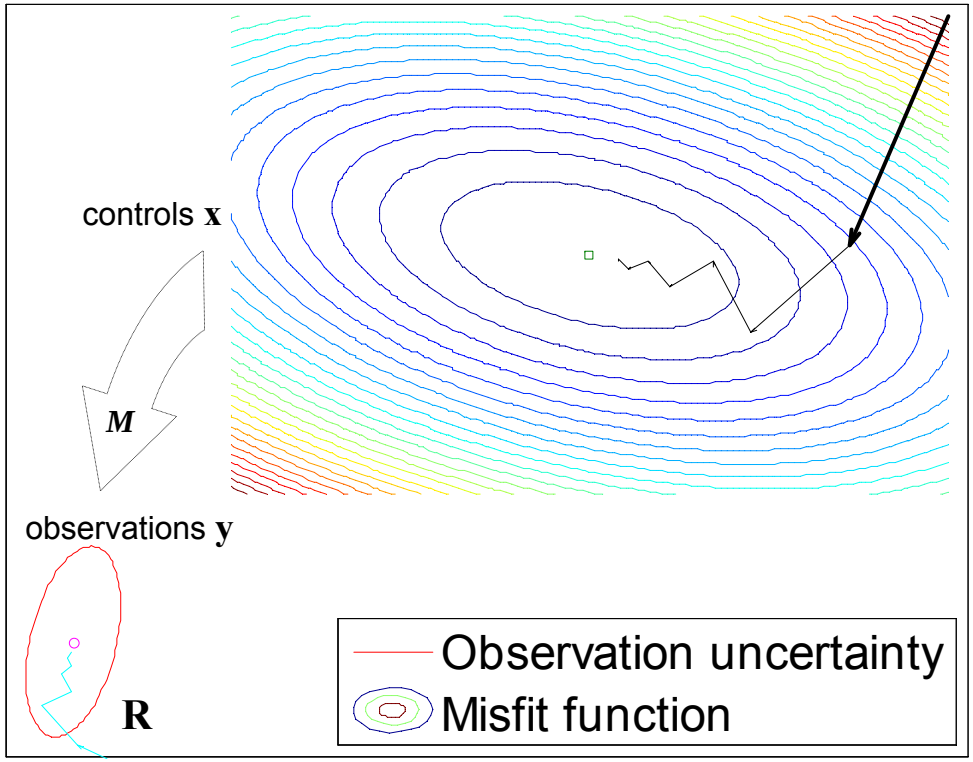
- **Method of Total Inversion** (Tarantola & Valette 1982)

Model–data misfit function: $J(\mathbf{x}) = \frac{1}{2}(\boldsymbol{M}(\mathbf{x}) - \mathbf{y})^T \mathbf{R}^{-1}(\boldsymbol{M}(\mathbf{x}) - \mathbf{y})$

– Weighted by data covariance: $\mathbf{R}$

Minimum of misfit function = Nonlinear least-squares solution $\hat{\mathbf{x}} = \arg\min_{\mathbf{x}} J(\mathbf{x})$

Gradient based optimization =
Adjoint method
(Method of Lagrange multipliers)



Solution uncertainty?

ECCO so far stops here …

Hessian method - uncertainty quantification

- Uncertainty of adjoint method solution → <u>curvature</u> of misfit function!

$$J(\mathbf{x}) = \tfrac{1}{2}(\boldsymbol{M}(\mathbf{x}) - \mathbf{y})^T \mathbf{R}^{-1}(\boldsymbol{M}(\mathbf{x}) - \mathbf{y})$$

- Described by **Hessian matrix** of J

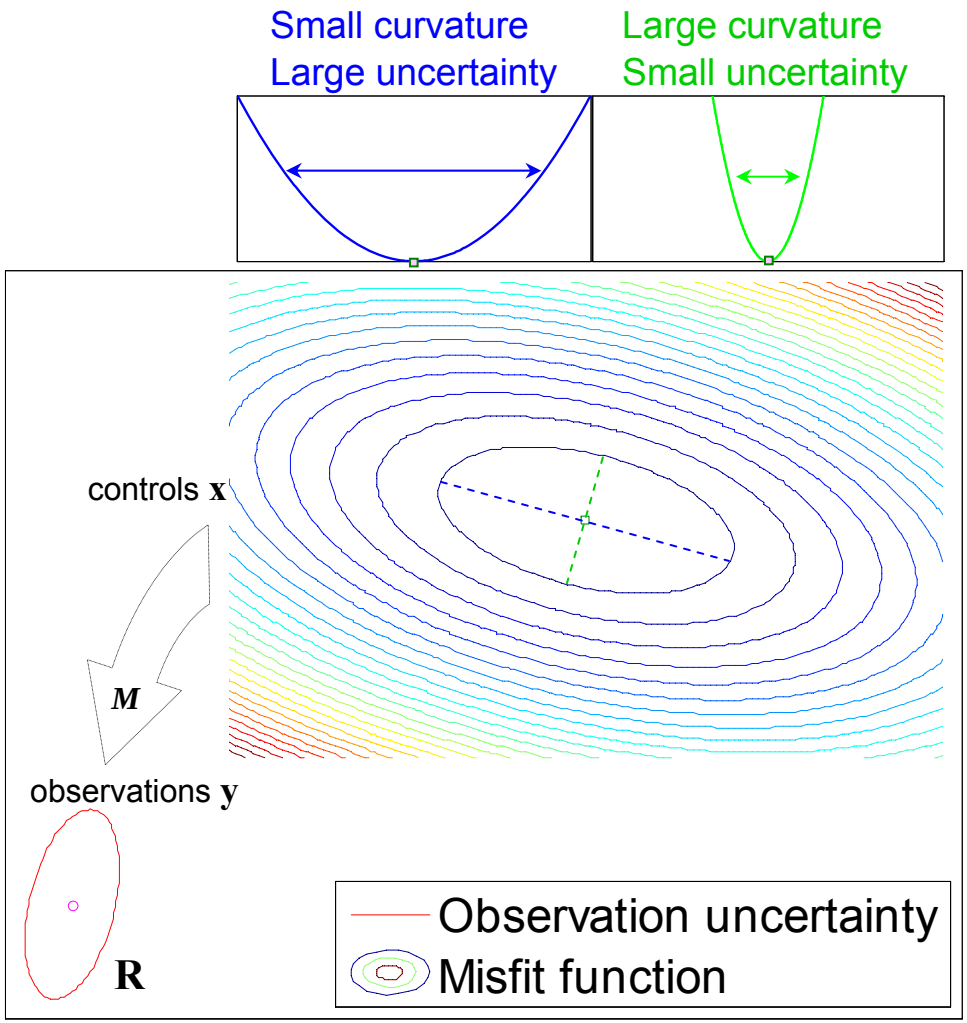
$$\mathbf{H} \equiv \frac{\partial^2 J}{\partial \mathbf{x}^2}(\hat{\mathbf{x}}) =$$

$$\underbrace{\left(\frac{\partial \boldsymbol{M}}{\partial \mathbf{x}^T}\right)^T \mathbf{R}^{-1}\left(\frac{\partial \boldsymbol{M}}{\partial \mathbf{x}^T}\right)}_{\text{Linear term}} + \underbrace{\left(\frac{\partial^2 \boldsymbol{M}}{\partial \mathbf{x}^2}\right)^T \mathbf{R}^{-1}\left(\boldsymbol{M}(\hat{\mathbf{x}}) - \mathbf{y}\right)}_{\text{Nonlinear term}}$$

For linear model or zero residual problem: **Hessian** is determined by product of model **Jacobians**

Posterior covariance of controls $\mathbf{x}$

≈ Inverse of Hessian matrix $\mathbf{P} \approx (\mathbf{H})^{-1}$



Hessian UQ methodology

- Adjoint method (first derivative)
  - State estimation

Data → Controls

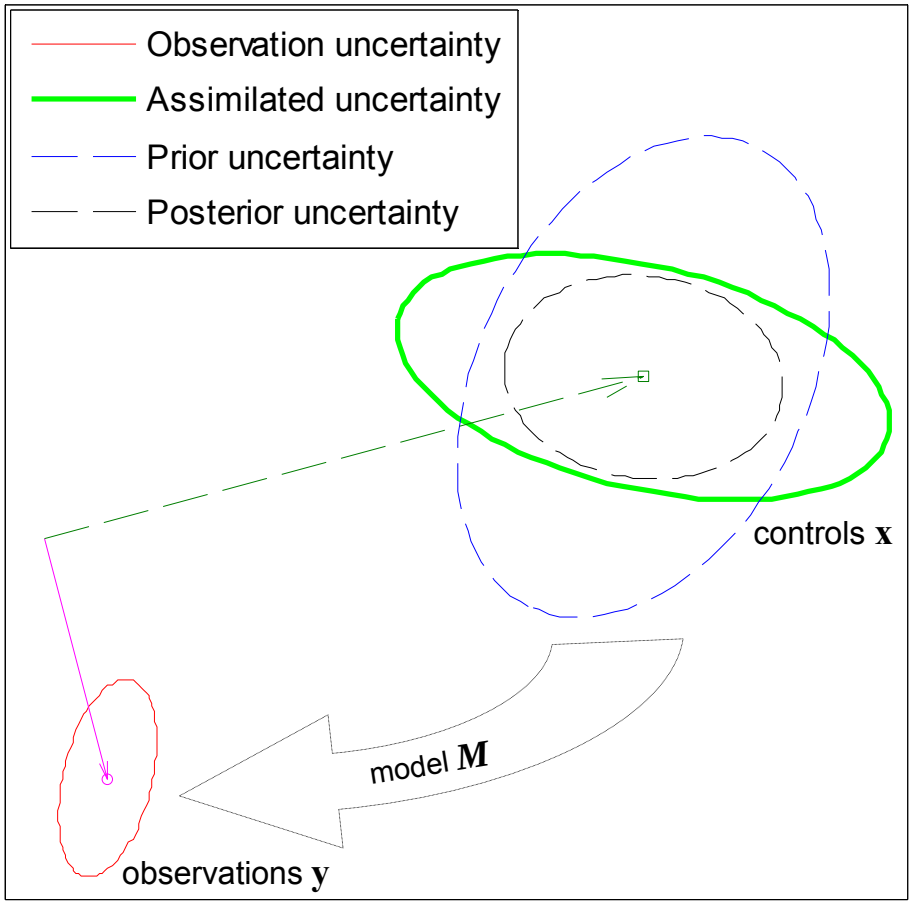
$\mathbf{y} \rightarrow \mathbf{x}$

- Hessian method (second derivative)
  - Uncertainty quantification

Data uncertainty → Controls uncertainty

$\mathbf{P}_{yy} \rightarrow \mathbf{P}_{xx}$

Invertible (well-posed) forward model



- Assimilation of observation uncertainty

$\mathbf{R} \rightarrow \mathbf{P}_{xx} = (\mathbf{H})^{-1}$

not exist for ill-posed problems

- Reduction of prior controls uncertainty

$\mathbf{P}_0$ and $\mathbf{P}_{xx} \rightarrow \mathbf{P} = \left(\mathbf{H} + \mathbf{P}_0^{-1}\right)^{-1}$

Uncertainty assimilation for ill-posed problem

❖ Forward model not invertible

- Assimilation of observation uncertainty

$\mathbf{R} \not\rightarrow \mathbf{P}_{\mathbf{xx}} = (\mathbf{H})^{-1}$ *singular matrix inversion, ill-conditioned inversion*

- Prior-to-posterior uncertainty reduction

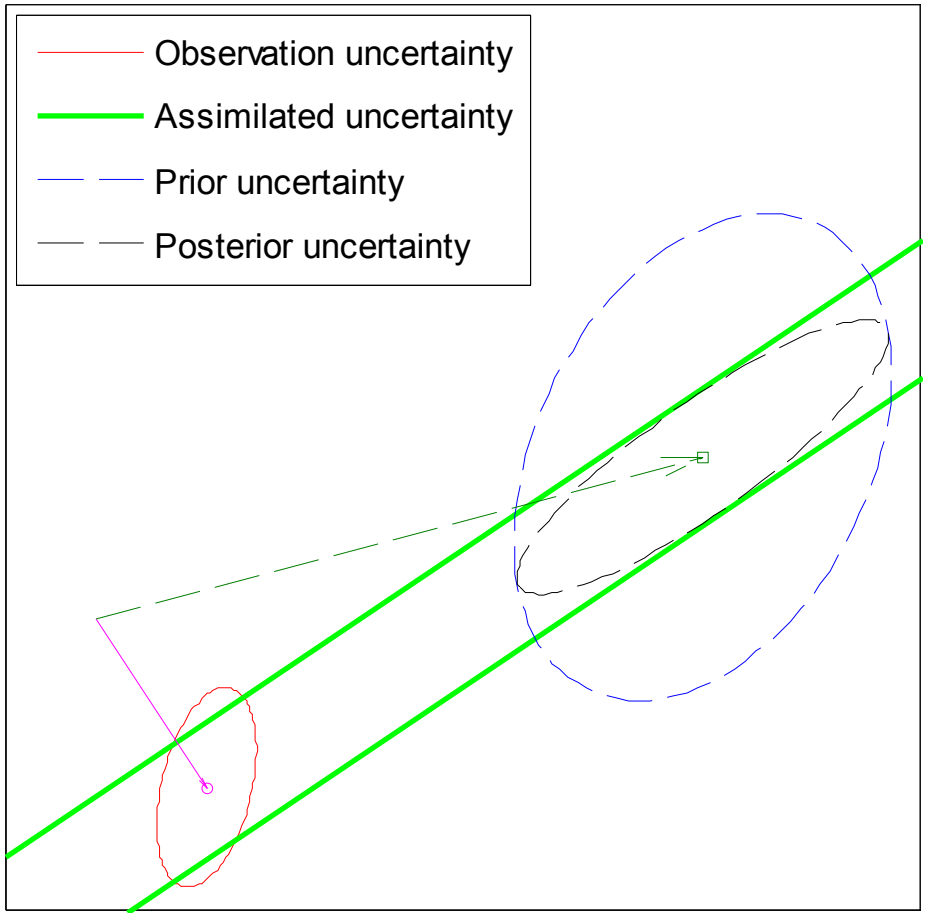
$\mathbf{P}_0$ and "$\mathbf{P}_{\mathbf{xx}}$" $\rightarrow$ $\mathbf{P} = \left(\mathbf{H} + \mathbf{P}_0^{-1}\right)^{-1}$

- Hessian spectral decomposition:

$$\mathbf{H} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T = \sum_i \lambda_i \mathbf{v}_i \mathbf{v}_i^T$$

- Hessian **Nullspace** $\{\mathbf{v}_i \mid \lambda_i = 0\}$
  - not constrained by data
  - infinite uncertainty
- Hessian **Range** $\{\mathbf{v}_i \mid \lambda_i \neq 0\}$
  - data-supported sub-domain
  - finite uncertainty constrained by data

➢ use nullspace to compress Hessian inversion



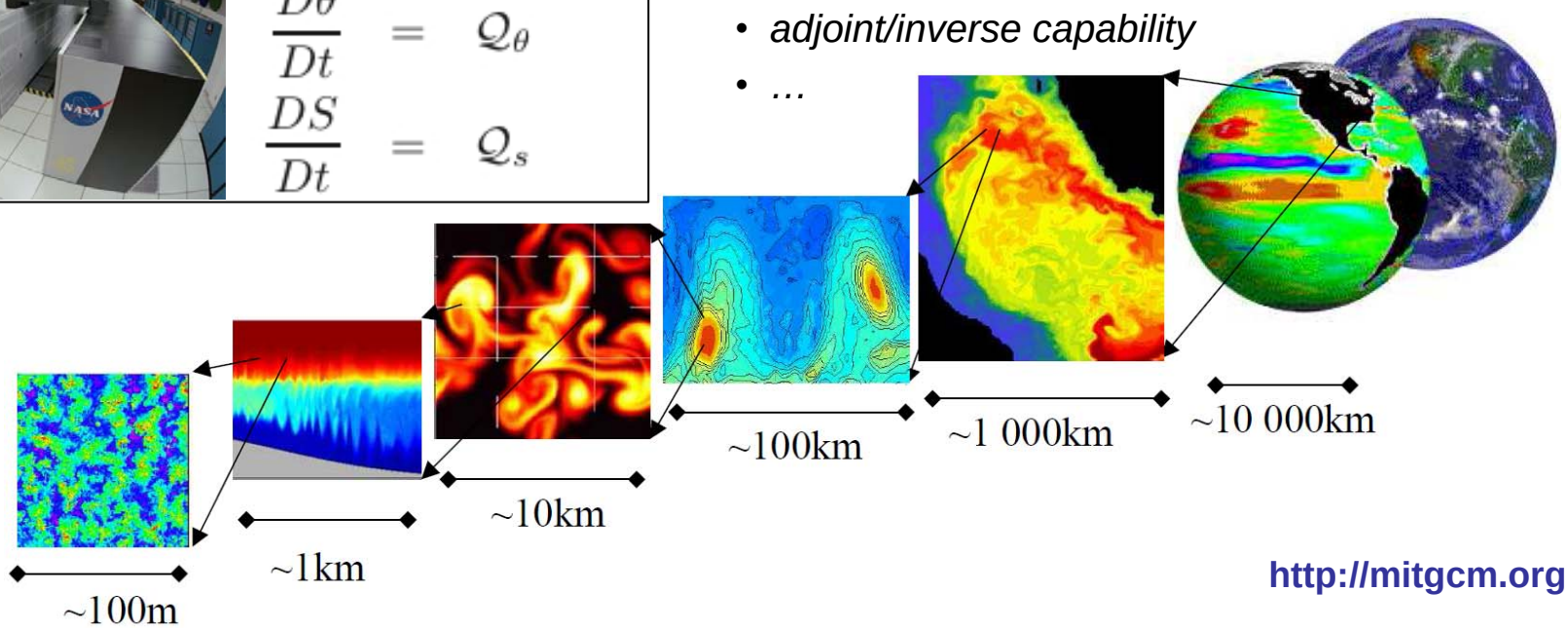
Implementation in MIT general circulation model (MITgcm)

- Key technical achievement
- Simplified configuration (2D, not all parameterizations)

$$
\begin{aligned}
\frac{D\vec{\mathbf{v}}_h}{Dt} + f\hat{\mathbf{k}} \times \vec{\mathbf{v}}_h + \frac{1}{\rho_c}\nabla_z p &= \vec{\mathcal{F}} \\
\epsilon_{nh}\frac{Dw}{Dt} + \frac{g\rho}{\rho_c} + \frac{1}{\rho_c}\frac{\partial p}{\partial z} &= \epsilon_{nh}\mathcal{F}_w \\
\nabla_z \cdot \vec{\mathbf{v}}_h + \frac{\partial w}{\partial z} &= 0 \\
\rho &= \rho(\theta, S) \\
\frac{D\theta}{Dt} &= \mathcal{Q}_\theta \\
\frac{DS}{Dt} &= \mathcal{Q}_s
\end{aligned}
$$

Approximated form of Navier-Stokes equations for an incompressible fluid, consisting of:

- *momentum equation (including Coriolis term)*
- *conservation of mass (continuity equation)*
- *conservation of tracers (heat, salt)*
- *equation of state*
- *subgrid-scale parameterizations*
- *scalable (domain decomposition)*
- *general curvilinear grid (incl. cubed-sphere)*
- *adjoint/inverse capability*
- *…*



http://mitgcm.org

Hessian computation and inversion

- **A**lgorithmic **D**ifferentiation (**AD**) of Fortran code
  - "forward-over-reverse" differentiation of adjoint code
- **Matrix-free** Hessian evaluation, Hessian-vector product code $\mathbf{H}\cdot\begin{bmatrix}0\\1\\0\\\vdots\\0\end{bmatrix}=col_2(\mathbf{H})$
- Lanczos matrix-free eigendecomposition
- Large matrix – $O(10^{10})$ elements, O(60GB) of storage

Matrix inversion dimensionality reduction:

Control space >> independent observations with nonzero information

$\dim(\mathbf{H}) >> \mathrm{rank}(\mathbf{H})$

$O(10^5)$ >> $O(100)$

→ *Details in Kalmikov and Heimbach (submitted to SISC, 2013)*

- Direct differentiation with AD!
  - **Hessian code**

→ Required for nonlinear and large residual problems

- Linearized Hessian
  - **Jacobian code**

$$\mathbf{H}_L=\left(\frac{\partial \boldsymbol{M}}{\partial \mathbf{x}^T}\right)^T \mathbf{R}^{-1}\left(\frac{\partial \boldsymbol{M}}{\partial \mathbf{x}^T}\right)$$

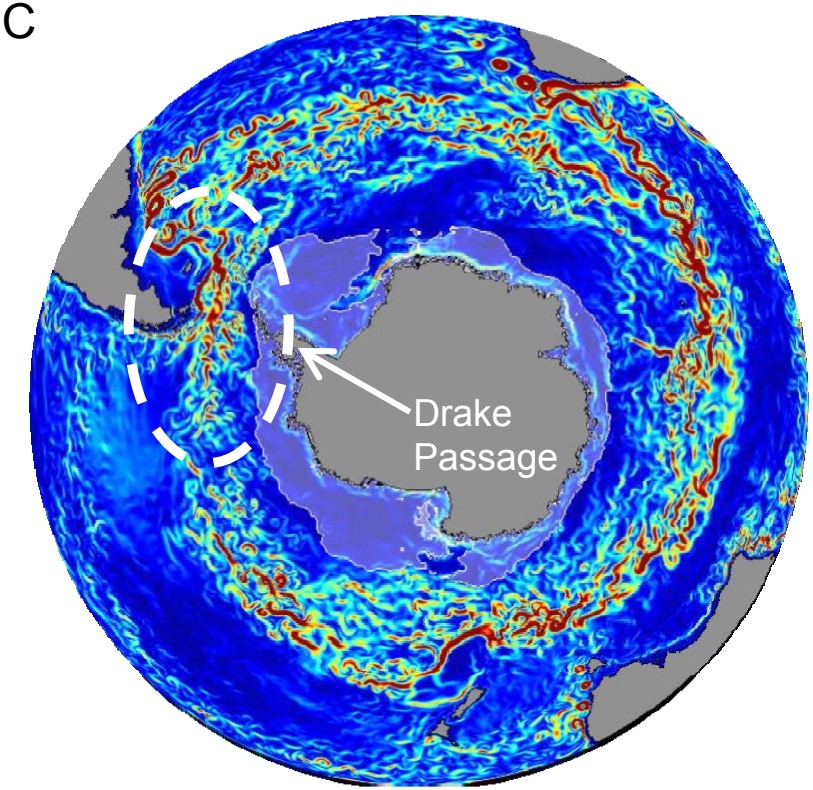
- Low rank Hessian approximation
  - **Adjoint code**

Antarctic Circumpolar Current (ACC) Transport

- Drake Passage – the narrowest constriction of ACC

- Mass transport in Southern Ocean
  - Important oceanographic index
  - Common modeling metric

- Simplified modeling in barotropic framework

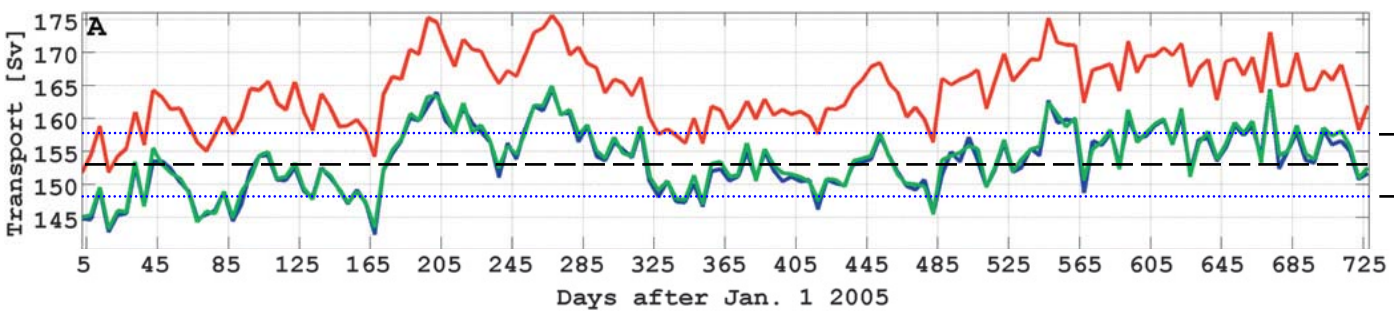


Southern Ocean State Estimation (SOSE)
Mazloff, Heimbach and Wunsch (2010)

- Ad-hoc uncertainty estimates:
- ➢ **Standard deviations of temporal variability**

→ *Need:* **Formal** uncertainty measure based on uncertainties of observations and modeling

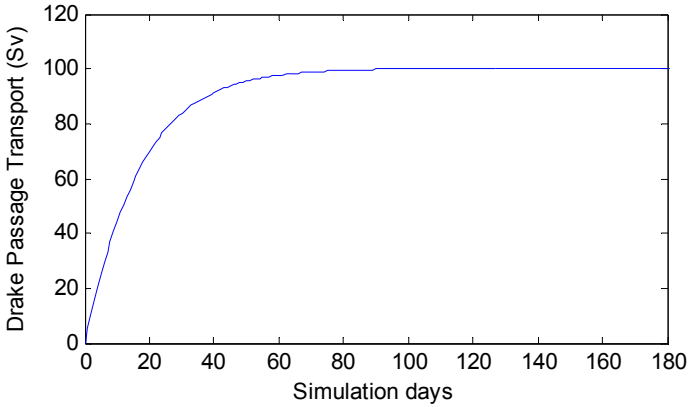
- SOSE Drake Passage transport estimate: 153 ± 5 Sv (Sv = 10^6 m^3/s)

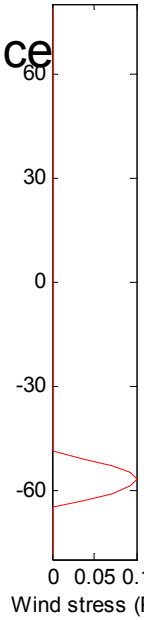


$$\sigma_{\text{variability}}(T) = \sqrt{\left\langle \left(T - \langle T \rangle\right)^2 \right\rangle}$$

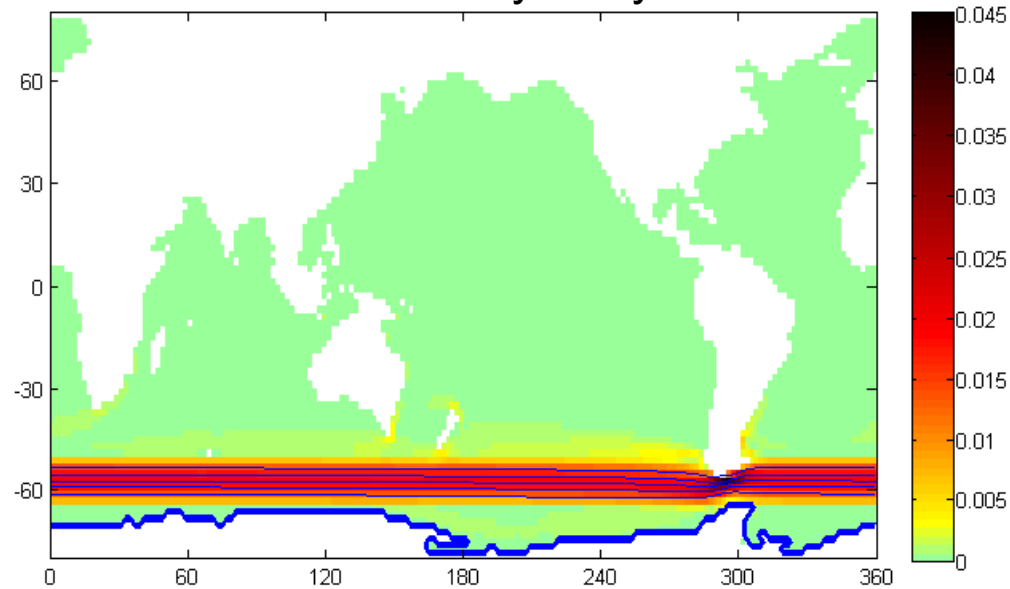
MITgcm modeling of ACC

- Barotropic configuration
- Wind forcing – Bottom drag balance
- Drake Passage transport

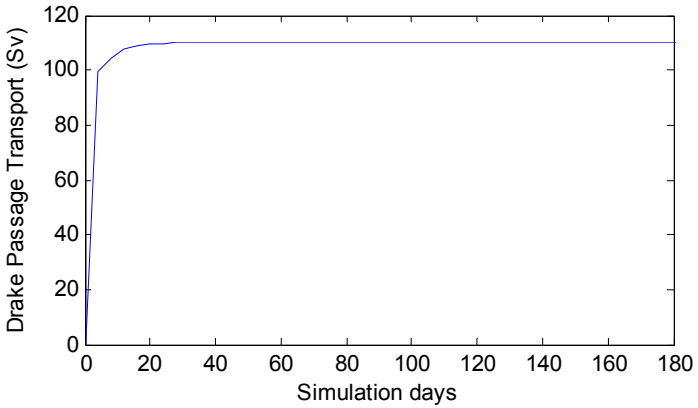


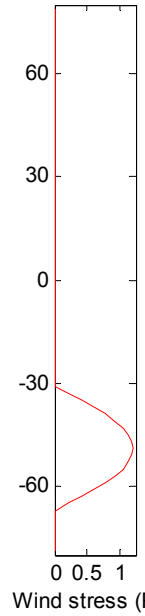


Flat bathymetry

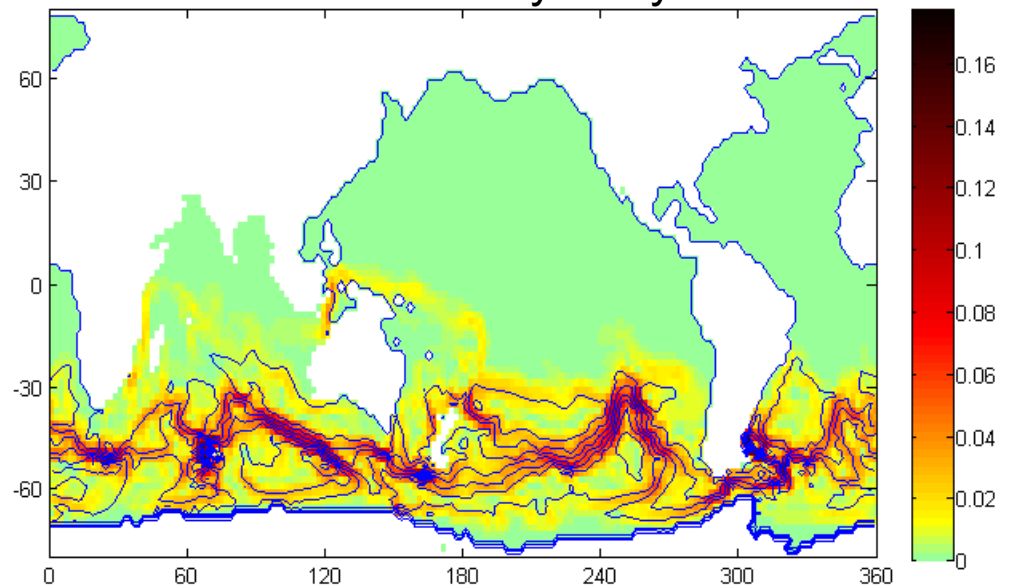


- Constrained by bottom topography
- Flow follows geostrophic contours
- Faster adjustment to steady state





Real bathymetry



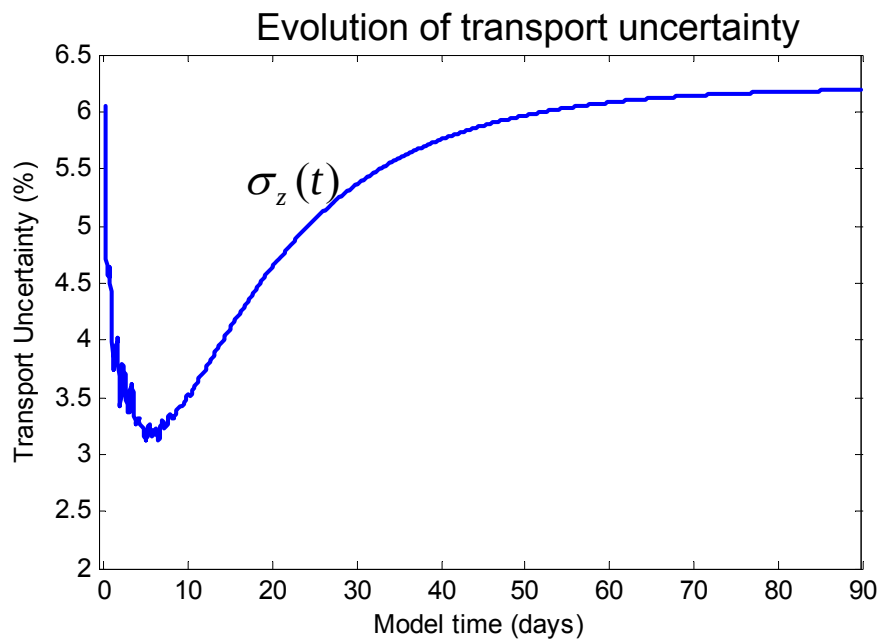
Forward uncertainty propagation

Controls uncertainty → Target uncertainty
$\Delta\mathbf{x}$ → $\Delta\mathbf{z}$

Covariance propagation: $$\sigma_z^2(t) = \left(\frac{\partial N}{\partial \mathbf{x}^T}\right)\mathbf{P}_{\mathbf{xx}}\left(\frac{\partial N}{\partial \mathbf{x}^T}\right)^T$$

- Nonlinear forward model: $z(t) = N(t, \mathbf{x})$
- Model controls: $\mathbf{x} = \left[\underbrace{\tau_x, \tau_y, r}_{\text{BC}}, \underbrace{u_0, v_0, \eta_0}_{\text{IC}}\right]^T$

  (initial & boundary conditions)



- Time dependent model
- Time dependent model derivatives
- Time dependent model uncertainty

A priori control uncertainty:

- correlations unknown
- assume independent **prior uncertainties**

Diagonal prior covariance:

$$\mathbf{P}_{\mathbf{xx}} = \mathbf{P}_0 = \begin{bmatrix} \sigma_{x_1}^2 & 0 & 0 \\ 0 & \sigma_{x_2}^2 & 0 \\ 0 & 0 & \sigma_{x_3}^2 \end{bmatrix}$$

Quadrature rule: $$\sigma_z^2 = \sum_i \left(\frac{\partial N}{\partial x_i}\right)^2 \sigma_{x_i}^2 + \cancel{\sum_i \sum_{j \neq i} \frac{\partial N}{\partial x_i}\frac{\partial N}{\partial x_j}\sigma_{x_i}\sigma_{x_j}\rho_{ij}}$$

- addition of independent uncertainties

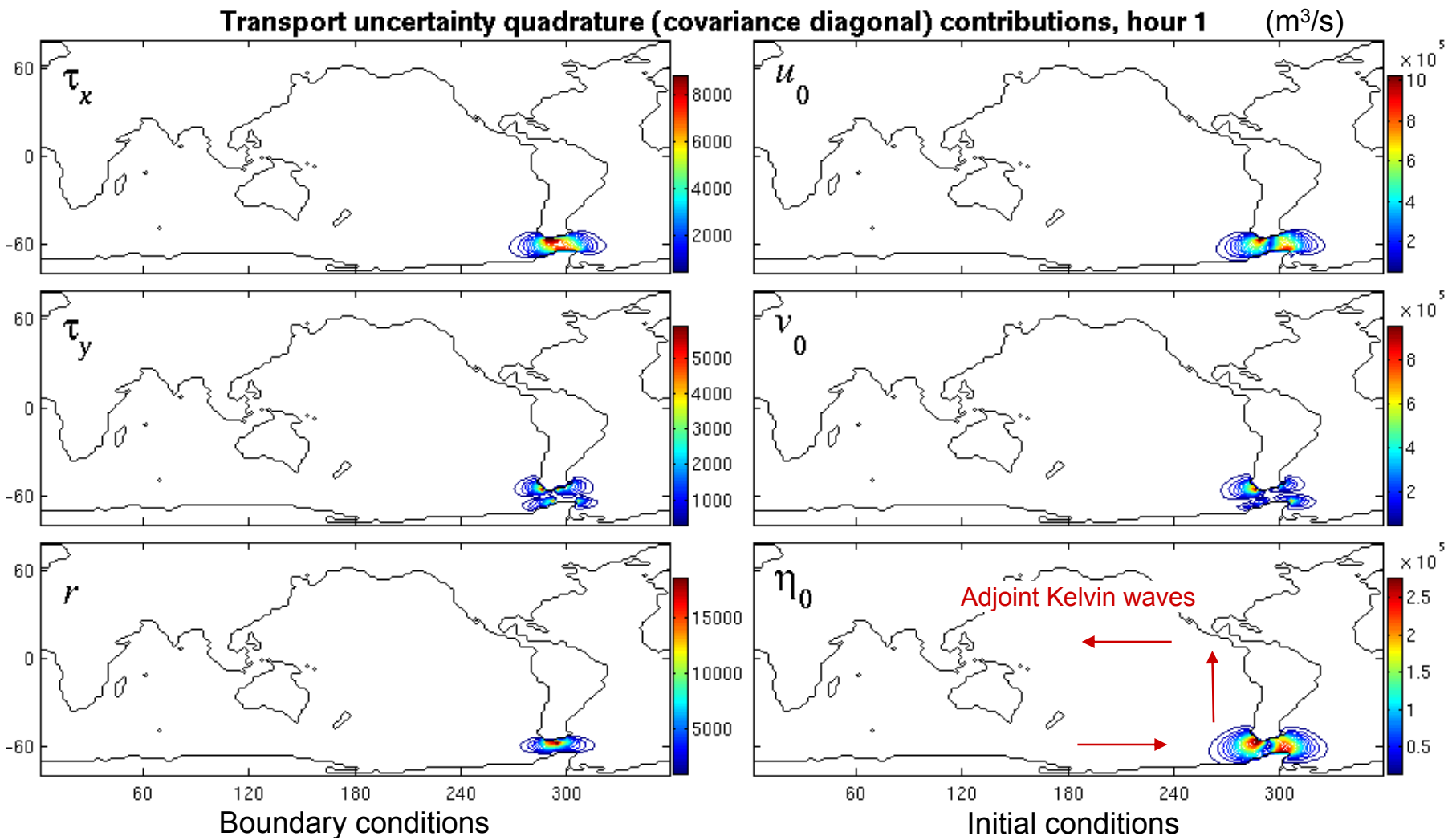
Uncertainty propagation mechanisms

Quadrature sum: $\sigma_z^2 = \sum_i \left(\frac{\partial N}{\partial x_i} \sigma_{x_i} \right)^2$

Control fields map

Wind Forcing X	Current Velocity U
Wind Forcing Y	Current Velocity V
Bottom Drag	Surface Elevation

- **Uncertainty waves**
- Reverse (adjoint) dynamics
- Adjoint Kelvin (gravity) waves



Uncertainty propagation mechanisms

Quadrature sum: $\sigma_z^2 = \sum_i \left(\frac{\partial N}{\partial x_i} \sigma_{x_i} \right)^2$

Control fields map

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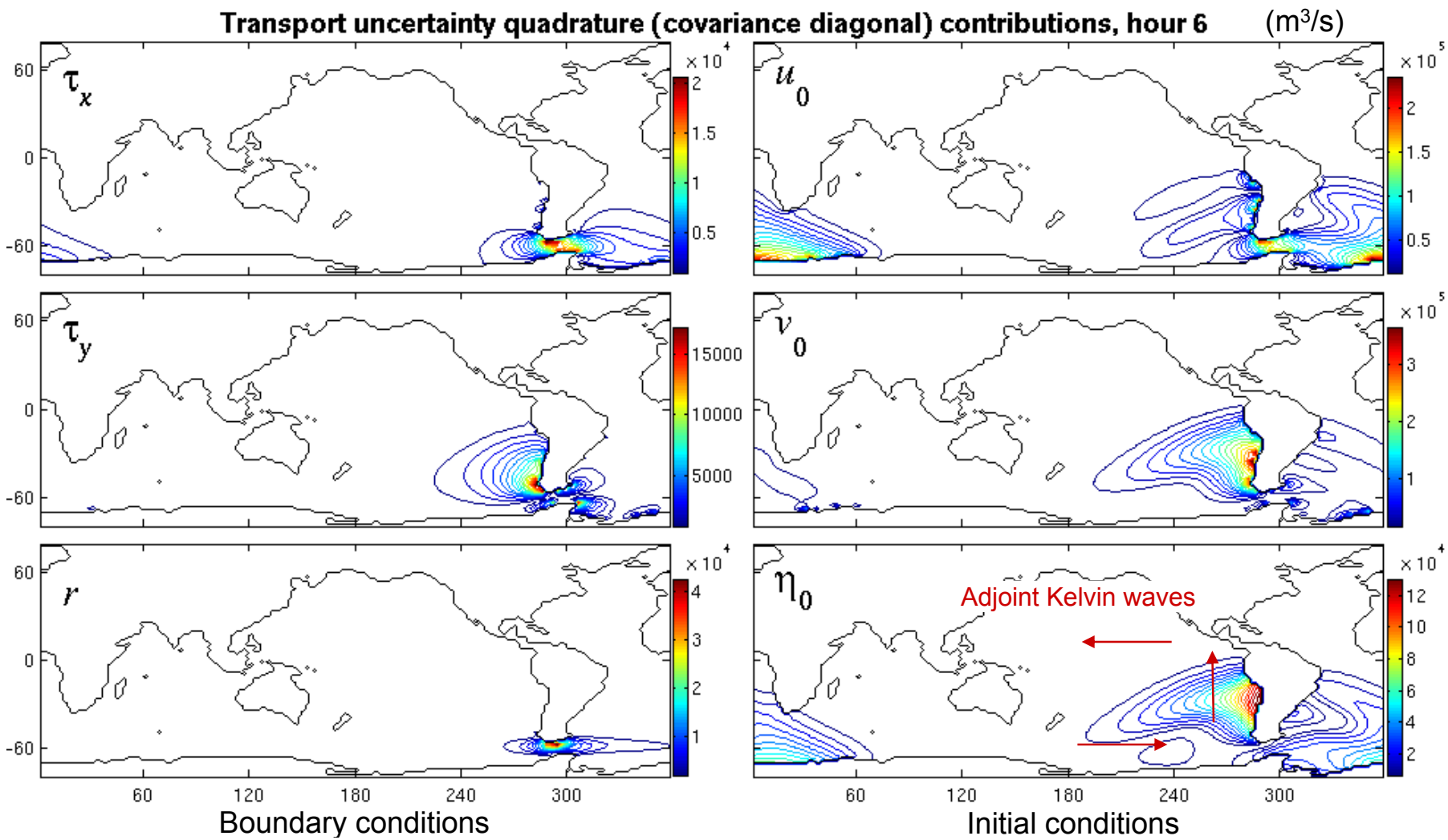
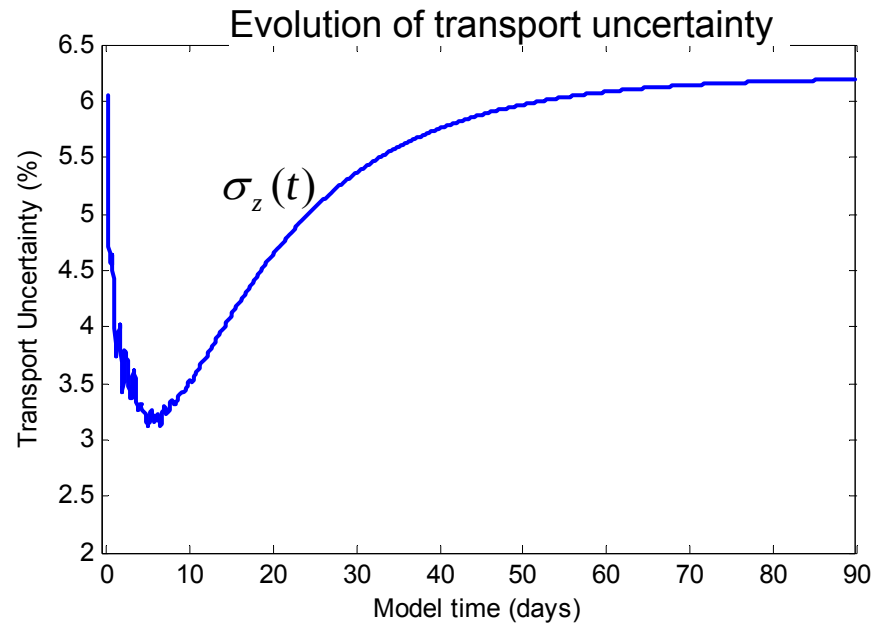


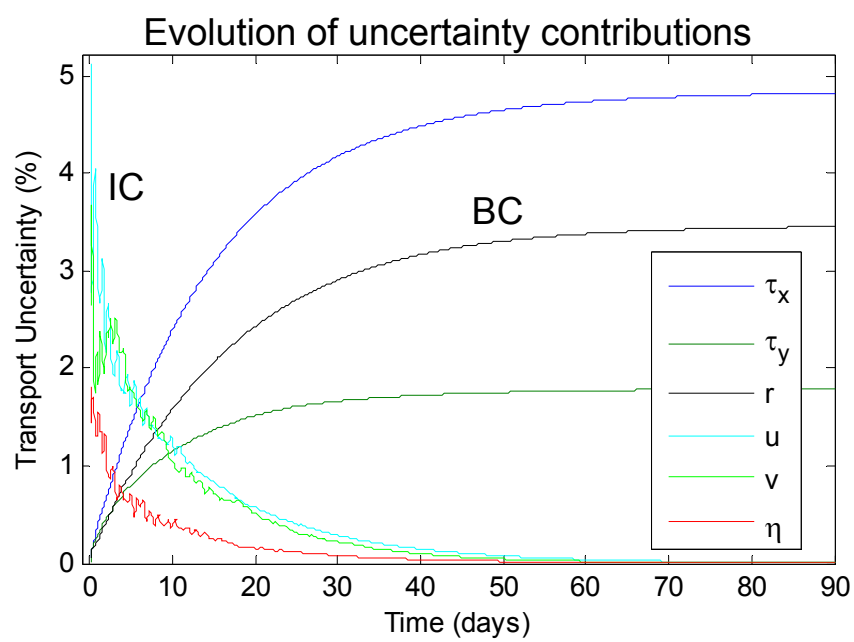
Forward uncertainty propagation dynamics

Covariance propagation: $\sigma_z^2(t) = \left(\frac{\partial N}{\partial \mathbf{x}^T}\right)\mathbf{P}_{\mathbf{xx}}\left(\frac{\partial N}{\partial \mathbf{x}^T}\right)^T$



Understanding the dynamics of uncertainty evolution

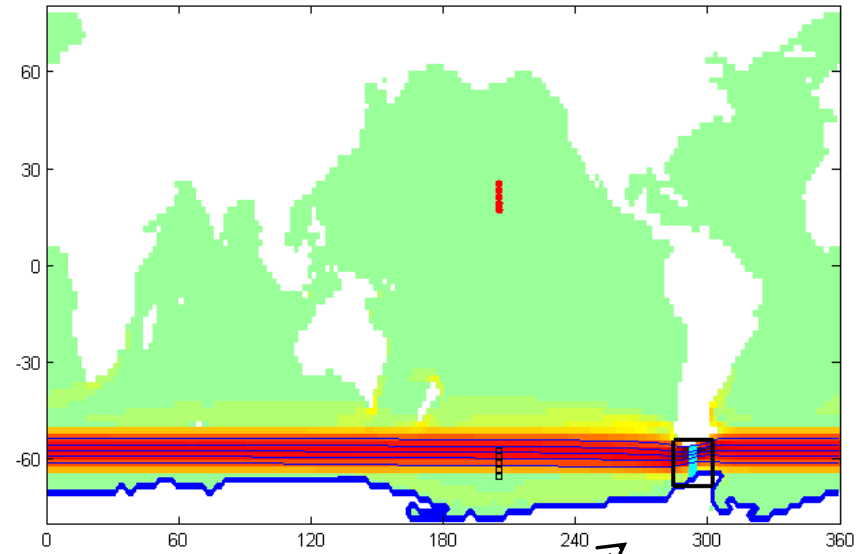
- Transport uncertainty due to **Initial Conditions** decays
  - Transient effects
- Transport uncertainty due to **Boundary Conditions** grows
  - Stationary effects



Quadrature sum: $\sigma_z^2 = \sum_i \left(\frac{\partial N}{\partial x_i}\sigma_{x_i}\right)^2$

Uncertainty assimilation experiments

- *Different observation systems*
- *Locations and geographic coverage*
- *Assimilation times*
- *Number of data points*
- *Type of variables*
- *Different control priors*



- How sea surface elevation observations constrain the Drake Passage transport?
- Effects of the uncertainty of sea surface elevation measurements on the uncertainty of Drake Passage transport?

UQ algorithm schemes and time dependence

Data uncertainty → Controls uncertainty → Target uncertainty

$\mathbf{P}_{\mathbf{yy}}$ → $\mathbf{P}_{\mathbf{xx}}$ → σ_z^2

Pure Prior-independent UQ

$$\mathbf{R} \longrightarrow \boxed{\mathbf{P}_{\mathbf{xx}} = \left(\mathbf{H}\right)^{-1}} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_{\mathbf{xx}} \mathbf{g}$$

Prior-to-Posterior uncertainty reduction

$$\mathbf{R}(t_a) \longrightarrow \boxed{\begin{array}{l} \mathbf{P}_0 \\ \downarrow \\ \mathbf{P}(t_a) = \left(\mathbf{H} + \mathbf{P}_0^{-1}\right)^{-1} \end{array}} \begin{array}{l} \longrightarrow \sigma_z^2(t) = \mathbf{g}^T \mathbf{P}_0 \mathbf{g} \\ \longrightarrow \sigma_z^2(t_a, t) = \mathbf{g}^T \mathbf{P} \mathbf{g} \end{array}$$

Observation / Assimilation time t_a

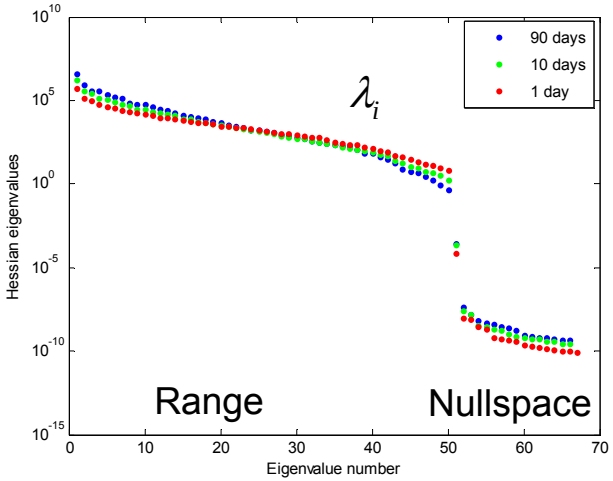
Forward propagation time t

Inverse uncertainty propagation (pure)

Hessian eigenvalue spectra

$$\mathbf{H} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T = \sum_i \lambda_i \mathbf{v}_i \mathbf{v}_i^T$$

- Spectral cut-off
- Estimation nullspace



$$\mathbf{R} \longrightarrow \boxed{\mathbf{P}_{xx} = (\mathbf{H})^{-1}} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_{xx} \mathbf{g}$$

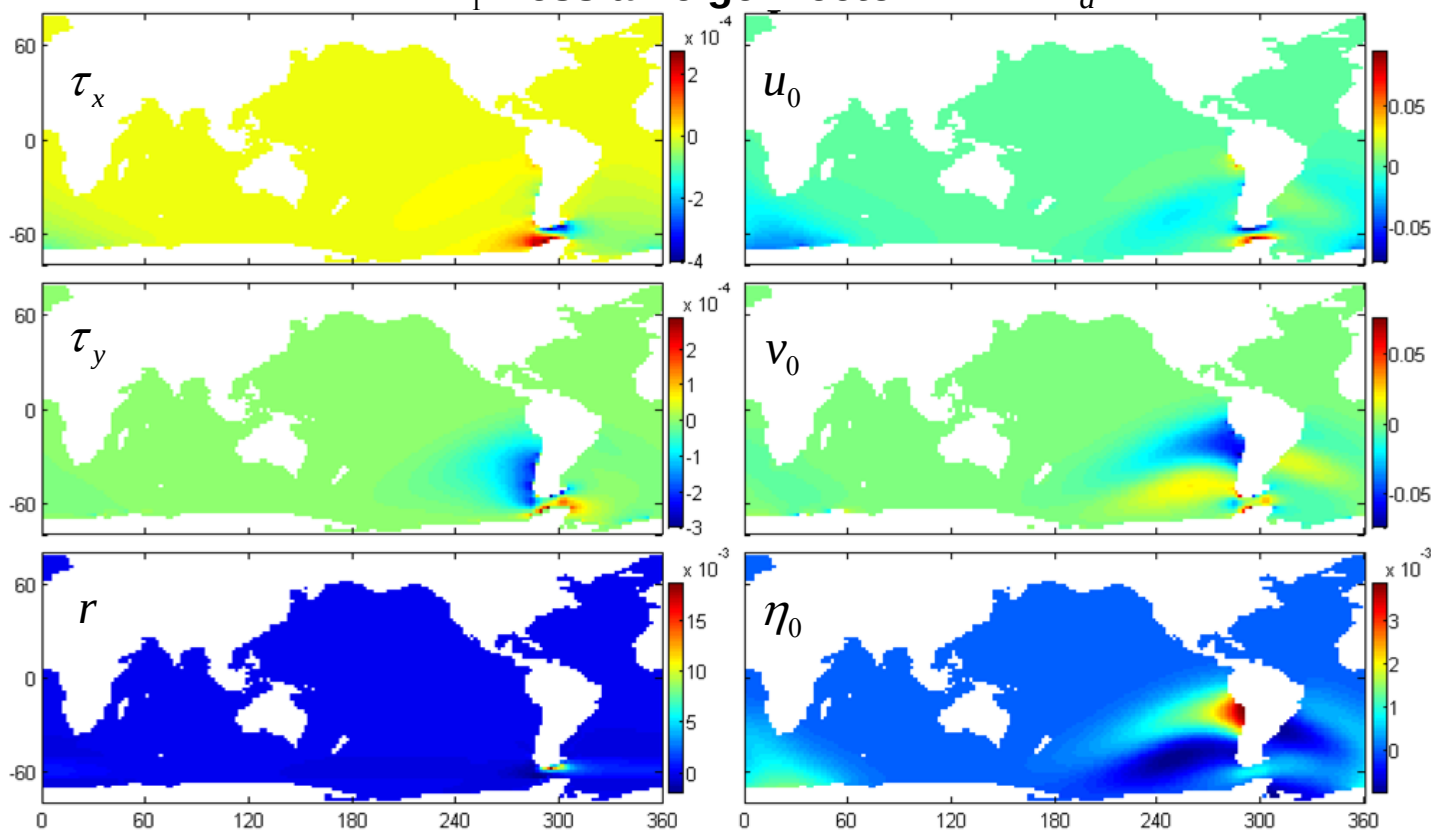
$$\mathbf{P}_0 \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_0 \mathbf{g}$$

$$\downarrow$$

$$\mathbf{R} \longrightarrow \mathbf{P} = \left(\mathbf{H} + \mathbf{P}_0^{-1}\right)^{-1} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P} \mathbf{g}$$

- Principal uncertainty patterns
- Wavy propagating structures
  - Hessian waves
  - Uncertainty waves!

$\mathbf{v}_1$ Hessian eigenvector 1 t_a= 6 hours



Model uncertainty reduction

- Constraining independent prior uncertainties

Relative Prior-to-Posterior Uncertainty Reduction

$$\frac{\sigma_{prior} - \sigma_{post}}{\sigma_{prior}} \cdot 100$$

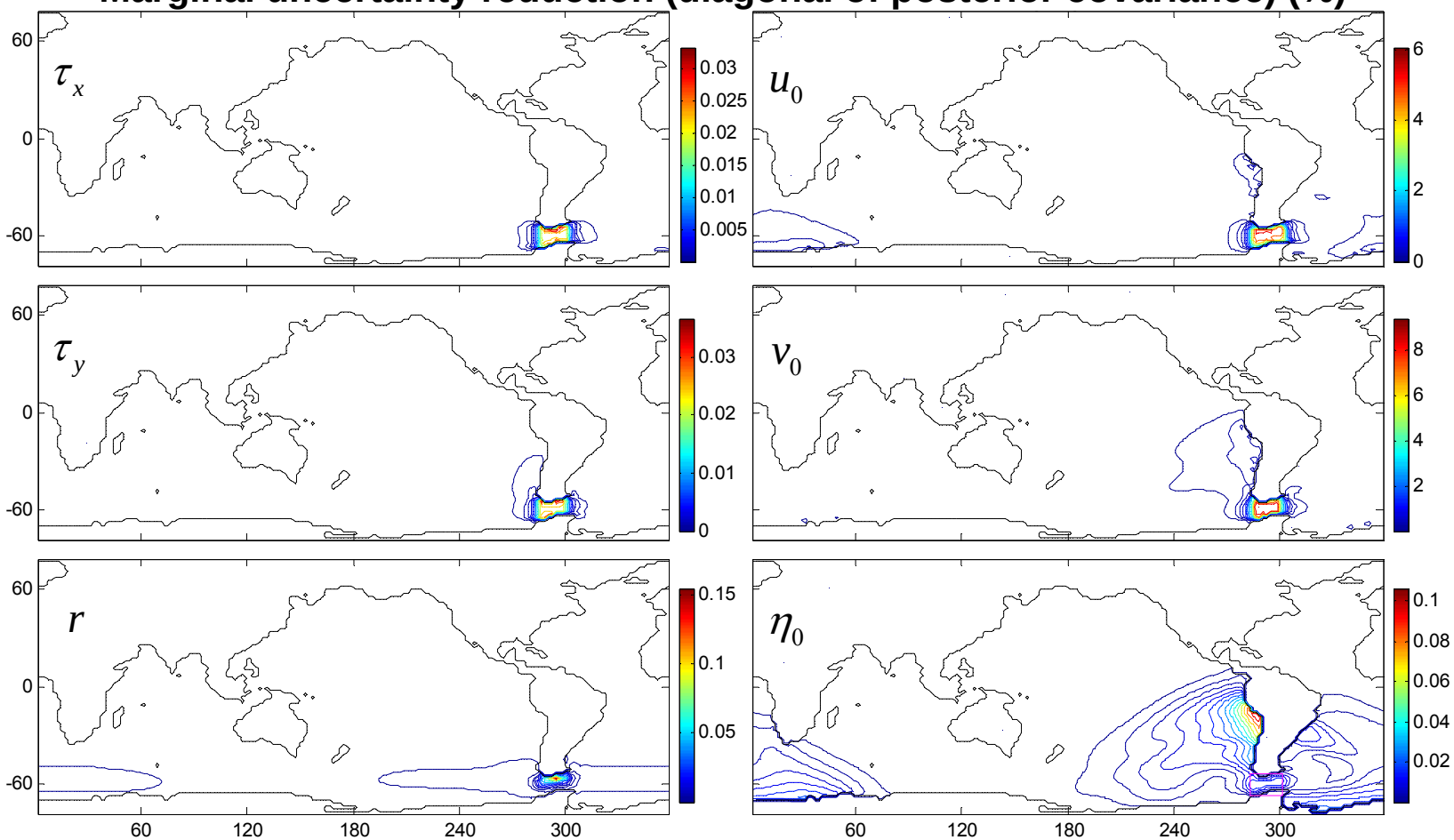
$$\mathbf{R} \longrightarrow \mathbf{P}_{xx} = (\mathbf{H})^{-1} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_{xx} \mathbf{g}$$

$$\mathbf{P}_0 \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_0 \mathbf{g}$$

$$\mathbf{R} \longrightarrow \mathbf{P} = \left(\mathbf{H} + \mathbf{P}_0^{-1}\right)^{-1} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P} \mathbf{g}$$

Marginal uncertainty reduction (diagonal of posterior covariance) (%)

t_a= 6 hours



Boundary conditions

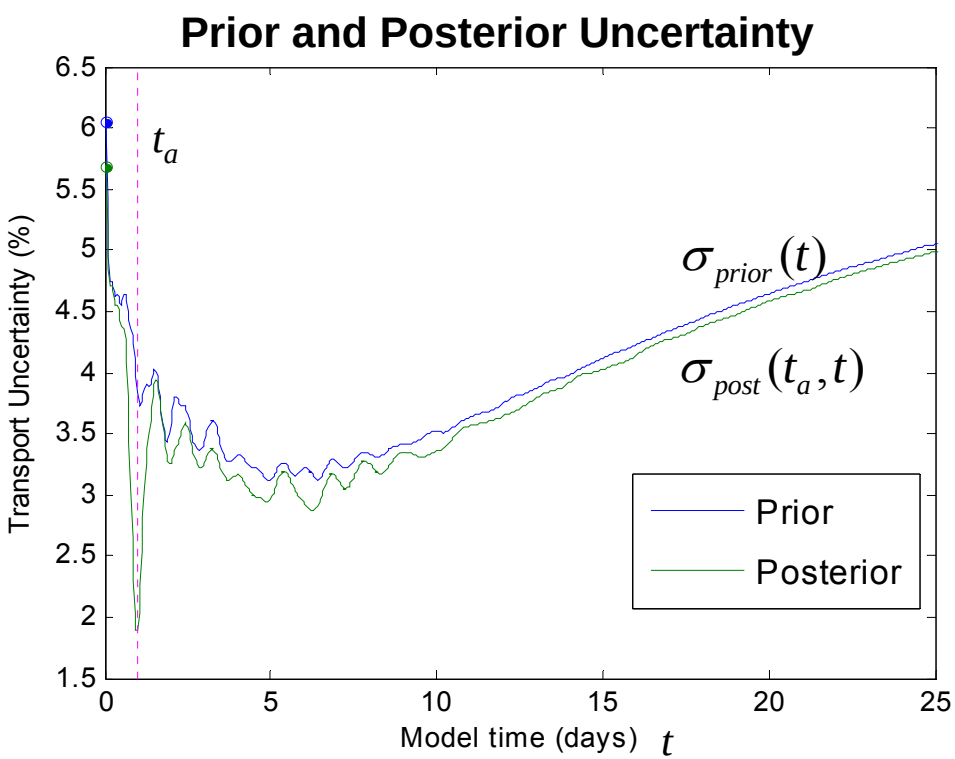
Initial conditions

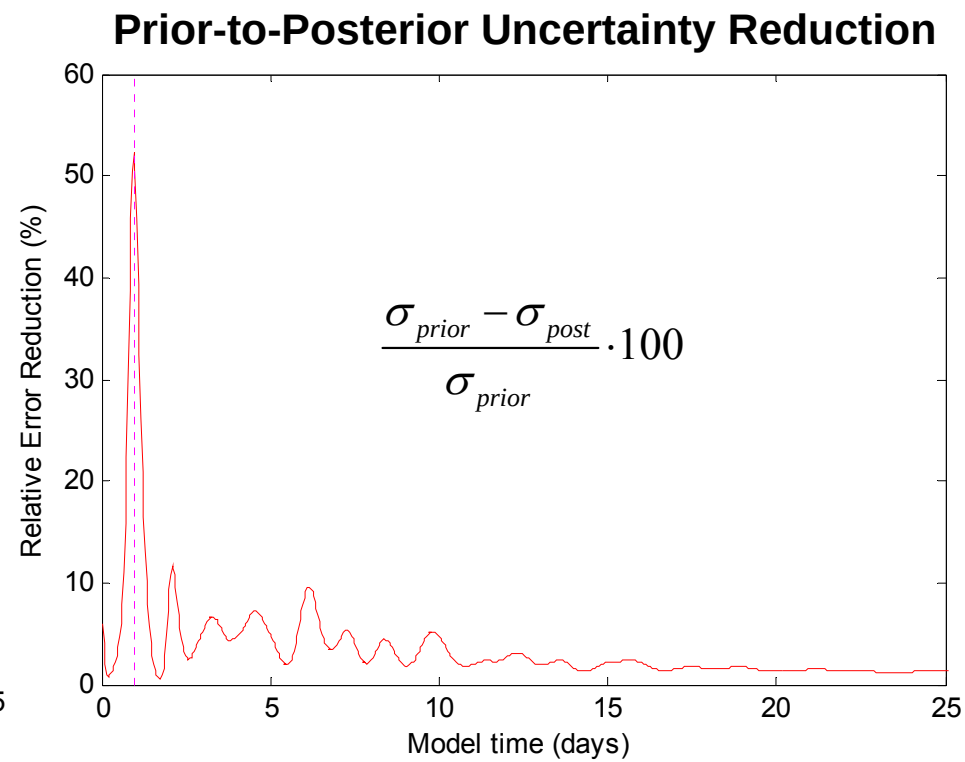
Forward uncertainty propagation & reduction

$$\begin{array}{ccccc} \mathbf{R} & \longrightarrow & \mathbf{P}_{xx} = (\mathbf{H})^{-1} & \longrightarrow & \sigma_z^2 = \mathbf{g}^T \mathbf{P}_{xx} \mathbf{g} \\ & & \mathbf{P}_0 & \longrightarrow & \boxed{\sigma_z^2 = \mathbf{g}^T \mathbf{P}_0 \mathbf{g}} \\ & & \downarrow & & \\ \mathbf{R} & \longrightarrow & \mathbf{P} = \left(\mathbf{H} + \mathbf{P}_0^{-1}\right)^{-1} & \longrightarrow & \boxed{\sigma_z^2 = \mathbf{g}^T \mathbf{P} \mathbf{g}} \end{array}$$

Uncertainty evolution of Drake Passage Transport

- **Time-resolving algorithm**
- Uncertainty assimilation on day 1 (t_a)
- **Transient** uncertainty reduction





Forward uncertainty propagation & reduction

$$\mathbf{R} \longrightarrow \mathbf{P}_{xx} = (\mathbf{H})^{-1} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_{xx} \mathbf{g}$$

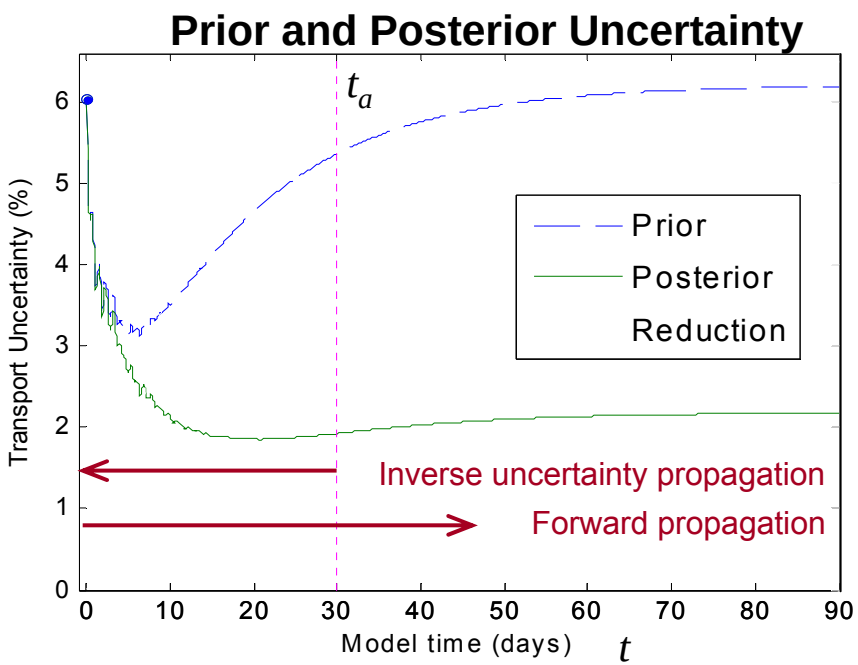
$$\mathbf{P}_0 \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_0 \mathbf{g}$$

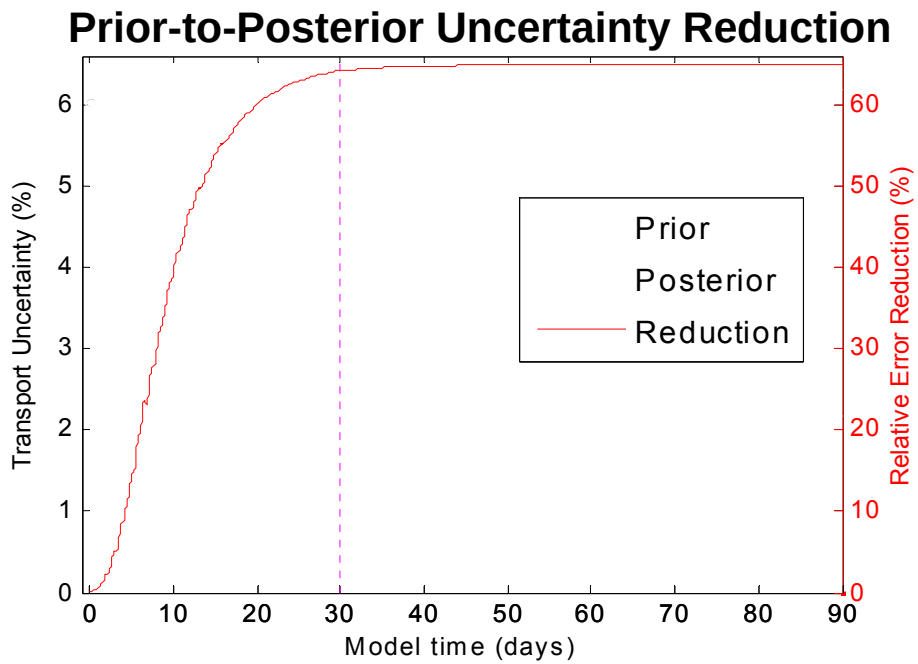
$$\downarrow$$

$$\mathbf{R} \longrightarrow \mathbf{P} = \left(\mathbf{H} + \mathbf{P}_0^{-1}\right)^{-1} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P} \mathbf{g}$$

Uncertainty evolution of Drake Passage Transport

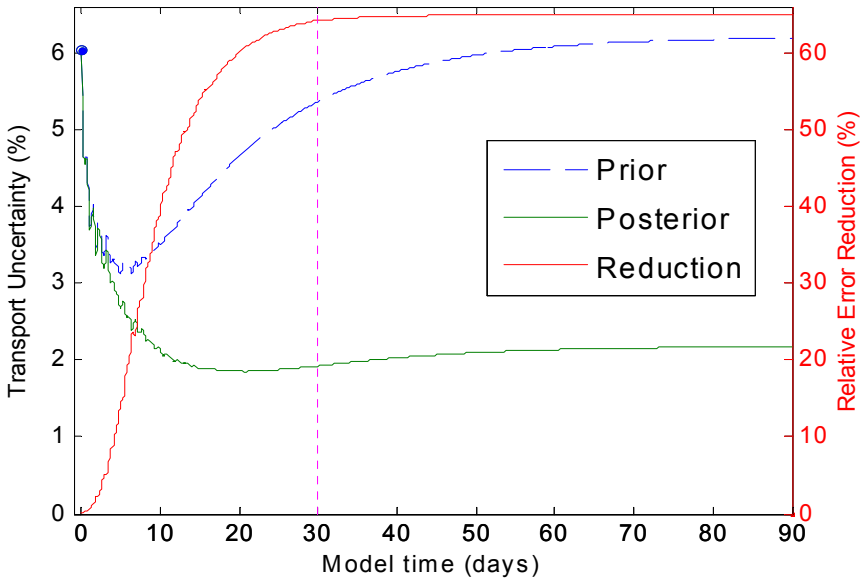
- **Time-resolving algorithm**
- Uncertainty assimilation on day 30 (t_a)
- **Stationary** uncertainty reduction

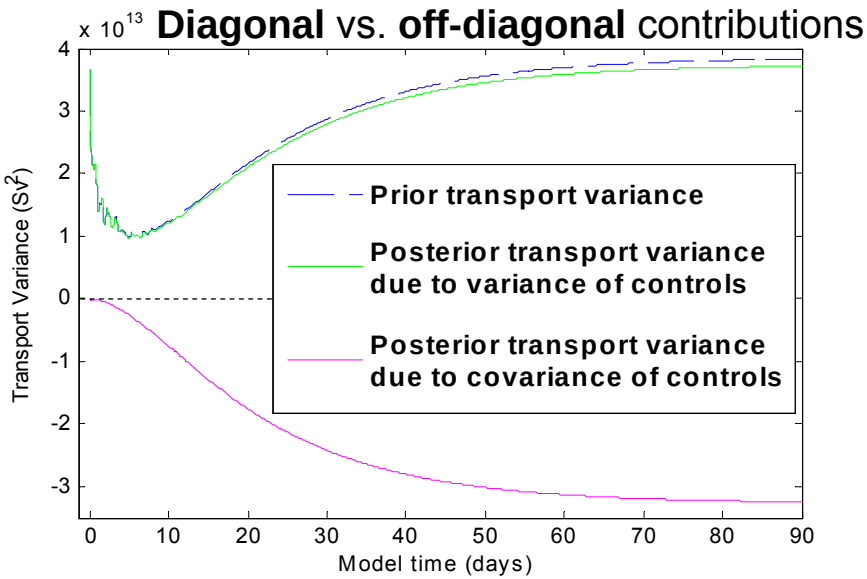




Posterior covariance coupling

- Uncertainty assimilation on day 30 (t_a)
- **Stationary** uncertainty reduction





$$\mathbf{R} \longrightarrow \mathbf{P}_{xx} = (\mathbf{H})^{-1} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_{xx} \mathbf{g}$$

$$\mathbf{P}_0 \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P}_0 \mathbf{g}$$

$$\mathbf{P}_0 \downarrow$$

$$\mathbf{R} \longrightarrow \mathbf{P} = \left(\mathbf{H} + \mathbf{P}_0^{-1}\right)^{-1} \longrightarrow \sigma_z^2 = \mathbf{g}^T \mathbf{P} \mathbf{g}$$

- **Diagonal** terms of posterior covariance
  vs.
- **Off-diagonal** terms of posterior covariance

$$\sigma_z^2 = \sum_i \left(\frac{\partial N}{\partial x_i}\right)^2 \sigma_{x_i}^2 + \sum_i \sum_{j \neq i} \frac{\partial N}{\partial x_i} \frac{\partial N}{\partial x_j} \sigma_{x_i} \sigma_{x_j} \rho_{ij}$$

- Observation uncertainty assimilation:
  - Reduces uncertainty of model controls (*small*)
  - Couples model controls (*large*)
- Correlations dominate uncertainty reduction of transport

Summary and conclusions

A significant step in development of **formal uncertainty quantification methodology** for large-scale ill-posed inverse problems:

- implemented a Hessian-based UQ framework within a global ocean state estimation system (**ECCO**)
- demonstrated for barotropic transport through Drake Passage within **MITgcm** and synthetic observations

Scalable numerical machinery

- **Inverse** and **Forward** uncertainty propagation
- Prior-independent UQ (pure) & prior-to-posterior uncertainty reduction (regularized UQ)
- **Range-nullspace** decomposition of estimation uncertainty
- Nonlinear AD **Hessian code**
- **Linearized** uncertainty description
- Depends on elimination of uncertainty **nullspace** when possible

Oceanographic insight

- Resolving **time evolution** of uncertainty - t**ransient** and s**tationary** uncertainty regimes
- Identifying the physical **mechanisms** of uncertainty dynamics (waves)
- Uncertainty **coupling** dominates uncertainty **reduction**

• **Next:** baroclinic high-resolution MITgcm with realistic forcing

Thank you!