Uncertainty Quantification as a Tool for Observing System Design An Oceanographic Perspective

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



Figure: OSNAP array of the Overturning in the Subpolar North Atlantic Program (http://www.o-snap.org)

OSNAP array:

• Deployed in summer 2014



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- Design based on dynamical considerations
- Review in 2020
- Data redundancy?

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- Potential for constraining remote quantities of interest (Qols)?





Figure: Submarine melt in Greenland's glacial fjords [Straneo and Heimbach, 2013]

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- Potential for constraining remote quantities of interest (Qols)?
 - e.g., Qol = subsurface temperature near Helheim Glacier

Inverse Modeling Framework (4D-Var): ECCO-V4 [Forget et al., 2015]

Final Goal:

Objectives:

Inverse Modeling Framework (4D-Var): ECCO-V4 [Forget et al., 2015]

- MITgcm at $\sim 1^{\circ} \times 1^{\circ}$ horizontal resolution, 50 vertical layers
- solves for uncertain initial conditions, time-evolving boundary conditions, parameters

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Objectives:

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- On the second second

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Nonlinear inverse/optimization problem (4D-Var): Minimize

$$\mathcal{J}(\mathbf{x}) = \frac{1}{2} [\underbrace{(\mathbf{y}^o - \mathcal{H}(\mathbf{x}))^T \mathbf{R}^{-1} (\mathbf{y}^o - \mathcal{H}(\mathbf{x}))}_{\text{weighted data-model misfit}} + \underbrace{(\mathbf{x} - \mathbf{x}^b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}^b)}_{\text{deviation from prior guess}}]$$



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Bayesian formulation of inverse problem:
$$\pi_{\text{post}}(\mathbf{x} | \mathbf{y}^{o}) \propto e^{-\mathcal{J}(\mathbf{x})} \approx \mathcal{N}(\mathbf{x}_{\text{MAP}}, \mathbf{P})$$



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$$\approx \mathbf{B}^{-1/2} \underbrace{(\sum_{i=1}^{M} \lambda_{i} \mathbf{v}_{i} \mathbf{v}_{i}^{T})}_{i=1} \mathbf{B}^{-1/2} \mathbf{D}$$
Uncertainty reduction for Qol
$$\sum_{i=1}^{M} \frac{\lambda_{i}}{\lambda_{i} + 1} \left\langle \mathbf{B}^{1/2} \frac{\partial \text{Qol}}{\partial \mathbf{x}}, \mathbf{v}_{i} \right\rangle^{2} \text{ data-constrained modes}$$

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$\{\boldsymbol{v}_i\}$ constrained by OSNAP heat transport measurements

West





West & East



West





West & East







East



West & East



West & East



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40°W

20°W



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 $\bm{B}^{1/2} \, \tfrac{\partial subT_{HG}}{\partial \bm{x}}$















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Outlook for redesign of OSNAP: Compute lowrank approximation via parallel randomized SVD methods [Halko et al., 2011]



References



1

Forget, G., Campin, J.-M., Heimbach, P., Hill, C. N., Ponte, R. M., and Wunsch, C. (2015).

ECCO version 4: an integrated framework for non-linear inverse modeling and global ocean state estimation. *Geosci. Model Dev.*, 8(10):3071–3104.

Halko, N., Martinsson, P. G., and Tropp, J. A. (2011).

Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions. SIAM Review, 53(2):217–288.

Straneo, F. and Heimbach, P. (2013).

North Atlantic warming and the retreat of Greenland's outlet glaciers. *Nature*, 504(7478):36–43.

Backup Slides

Low-rank approximation of misfit Hessian

$$\mathbf{P} = (\mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} + \mathbf{B}^{-1})^{-1}$$

linearized (or Gauss-Newton) Hessian

Misfit Hessian $\mathbf{H}_{\text{misfit}} = \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}$ is of low rank:

$$\tilde{\mathbf{H}}_{\text{misfit}} = \mathbf{B}^{1/2} \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \mathbf{B}^{1/2} \approx \sum_{i=1}^M \lambda_i \mathbf{v}_i \mathbf{v}_i^T$$

Expression for posterior covariance:

$$\mathbf{P} = \mathbf{B}^{1/2} \left(\tilde{\mathbf{H}}_{\text{misfit}} + \mathbf{I} \right)^{-1} \mathbf{B}^{1/2} = \mathbf{B}^{1/2} \left(\mathbf{I} - \sum_{i=1}^{M} \frac{\lambda_i}{\lambda_i + 1} \mathbf{v}_i \mathbf{v}_i^T \right) \mathbf{B}^{1/2}$$

$$= \mathbf{B} - \sum_{i=1}^{M} \frac{\lambda_i}{\lambda_i + 1} \left(\mathbf{B}^{1/2} \mathbf{v}_i \right) \left(\mathbf{B}^{1/2} \mathbf{v}_i \right)^T$$

Projection of weighted adjoint sensitivities - DS



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