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A Formulation of Forecast Error Covariance in High-Dimensional Ensemble Data Assimilation Suitable for State-Space Localization

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Motivation (1): Covariance localization

- *Covariance localization is necessary in high-dimensional ensemble and hybrid variational-ensemble data assimilation*
 - insufficient degrees of freedom from ensembles
 - state-space and observation-space localization
- *Observation-space localization*: increase observation error with distance from a central grid-point
 - Inconsistent for vertical localization when observations are vertically-integrated
 - Additional localization problem with observations impacting several components of a strongly-coupled modeling system
- *State-space localization*: apply Hadamard product between ensemble covariance and a pre-defined correlation matrix
 - Straightforward to apply vertical localization and to account for shared observations in a strongly-coupled systems

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Motivation (2): Bayesian inference

- Data assimilation is a recursive application of Bayes formula over time
- **The power of DA comes from Bayesian inference.** In DA practice Bayesian inference typically reduces to first two moments of a PDF (e.g., Gaussian PDF assumption)
- **VAR: Bayesian inference in terms of the first moment of a PDF.** No recursive estimation of forecast/analysis error covariance.
- **ENS: Bayesian inference in terms of the first and second moments of a PDF (mean, covariance).**
- **Hybrid ENS-VAR: Bayesian inference in terms of the first moment is kept, but Bayesian inference in terms of the second moment is broken!** Typically two separate DA systems, VAR and ENS. VAR produces the analysis, but the analysis error covariance estimate is from ENS and therefore corresponds to the ENS analysis.
- Therefore, **hybrid ENS-VAR** represents an **improvement of VAR**, but a **degradation of ENS** method

How to improve hybrid ENS-VAR?

- Estimate error covariance in hybrid ENS-VAR consistently with the analysis. This points to a need for a single system that does both the first and second moment estimation.
- Several benefits of hybrid ENS-VAR are generally noticed:
 - (1) Increased degrees of freedom result from combining static and ensemble error covariance
 - (2) Optimization/minimization is important for nonlinear processes and operators
 - (3) State-space covariance localization is advantageous for satellite observations.
- ENS has a formulation that allows Bayesian inference of the second PDF moment, but needs to address the above points.
- Advantages (1) and (2) have been addressed in ENS, but (3) is still a challenge.
- In this presentation we investigate a possibility for state-space covariance localization in ENS framework.

State-space square-root covariance localization used in current hybrid methods

Ensemble covariance is an outer product of ensemble perturbations

$$P_E = \sum_{i=1}^{N_e} p_i p_i^T \quad p_i = m(x_{t-1}^a + [p_i^a]_{t-1}) - m(x_{t-1}^a)$$

Localized error covariance is obtained as a Hadamard product with correlation L

$$L \circ P_E = L \circ \sum_{i=1}^{N_e} p_i p_i^T = \sum_{i=1}^{N_e} (L \circ p_i p_i^T)$$

Use Hadamard product identity ...

$$L \circ ab^T = \text{diag}(a) \cdot L \cdot \text{diag}(b)$$

... to obtain localized error covariance

$$L \circ P_E = \sum_{i=1}^{N_e} \text{diag}(p_i) \cdot L \cdot \text{diag}(p_i)$$

The square root localized forecast error covariance is

$$(L \circ P_E)^{1/2} = \left(D_1 L^{1/2} \quad \dots \quad D_{N_e} L^{1/2} \right) \quad D_i = \text{diag}(p_i)$$

New state-space localized covariance

Consider cost-function with localized forecast error covariance

$$J(x) = \frac{1}{2}(x - x^f)^T (L \circ P_E)^{-1} (x - x^f) + \frac{1}{2}[y - h(x)]^T R^{-1} [y - h(x)]$$

Embed identity matrix using random sample $N(0,1)$

$$(L \circ P_E) = (L \circ P_E)^{1/2} (L \circ P_E)^{T/2} = (L \circ P_E)^{1/2} I (L \circ P_E)^{T/2}$$

$$I \approx E[\varphi\varphi^T] = \frac{1}{N_r - 1} \sum_{j=1}^{N_r} \varphi_j \varphi_j^T$$

$$P_f = (L \circ P_E)^{1/2} \left[\frac{1}{N_r - 1} \sum_{j=1}^{N_r} \varphi_j \varphi_j^T \right] (L \circ P_E)^{T/2} = \frac{1}{N_r - 1} \sum_{j=1}^{N_r} [(L \circ P_E)^{1/2} \varphi_j] [(L \circ P_E)^{1/2} \varphi_j]^T$$

Use Hadamard product identity
to obtain **new forecast error covariance**

$$L \circ ab^T = \text{diag}(a) \cdot L \cdot \text{diag}(b)$$

$$P_f = \frac{1}{N_r - 1} \sum_{i=1}^{N_c} \sum_{j=1}^{N_r} [D_i L^{1/2} \varphi_j] [D_i L^{1/2} \varphi_j]^T$$

$$D_i = \text{diag}(p_i)$$

New square-root localized error covariance

$$F = (f_1 \quad \cdots \quad f_{N_c \times N_r}) \quad f_k = \frac{1}{\sqrt{N_r - 1}} D_i L^{1/2} \varphi_j \quad (k = 1, \dots, N_c \times N_r)$$

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Experimental setup

- Weather Research and Forecasting (WRF) model
- 27 km /31 layer
- 32 dynamical ensembles
- (1) 1024 and (2) 4096 random ensembles
- 6-hour forecast error covariance
- **Random:** use $D_i=I$ in localized covariance formulation
- **Total:** use complete localized covariance formulation
- Single observation experiment

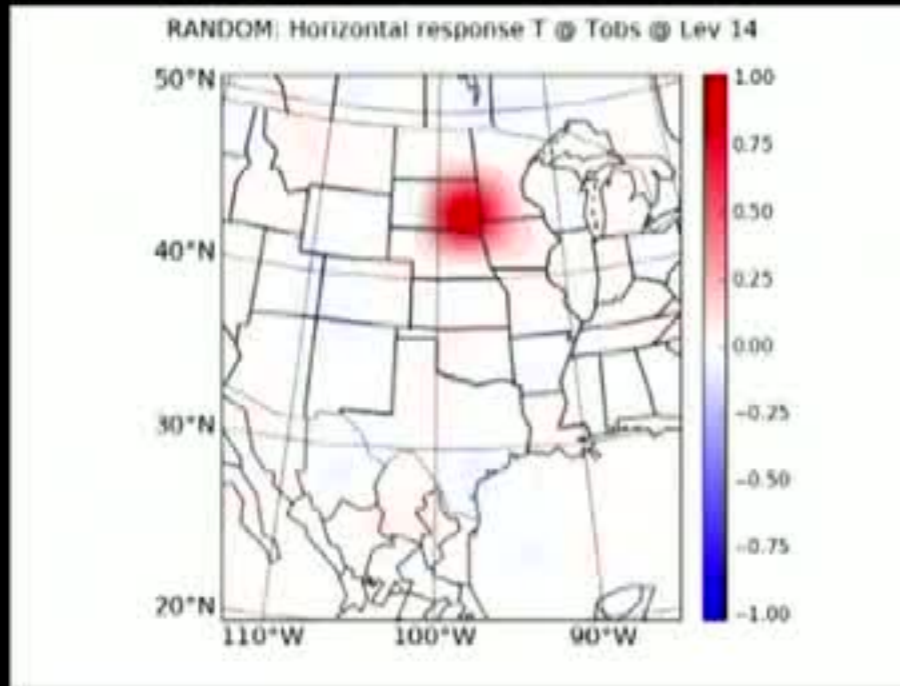
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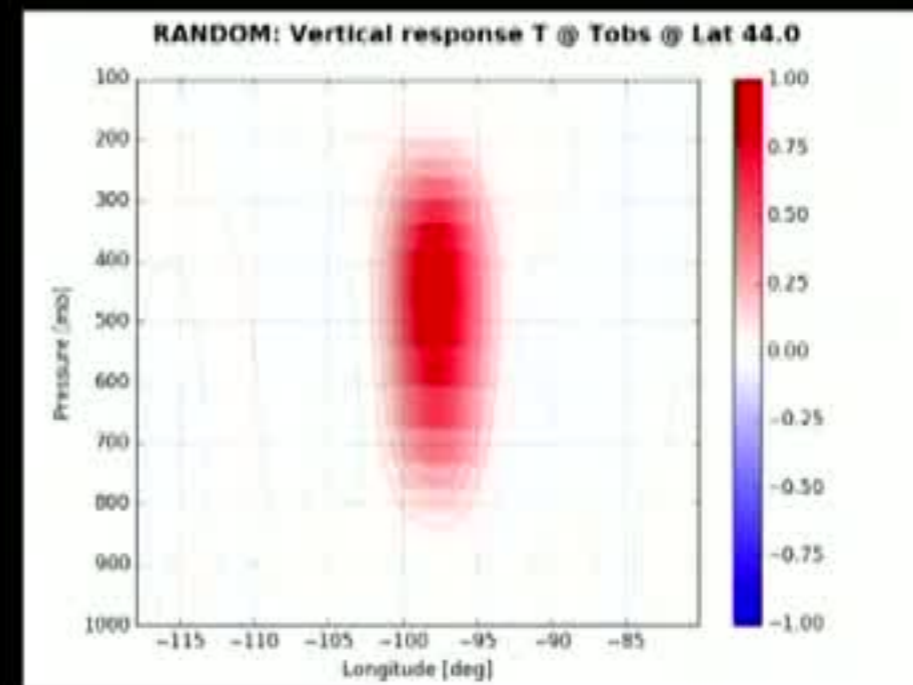
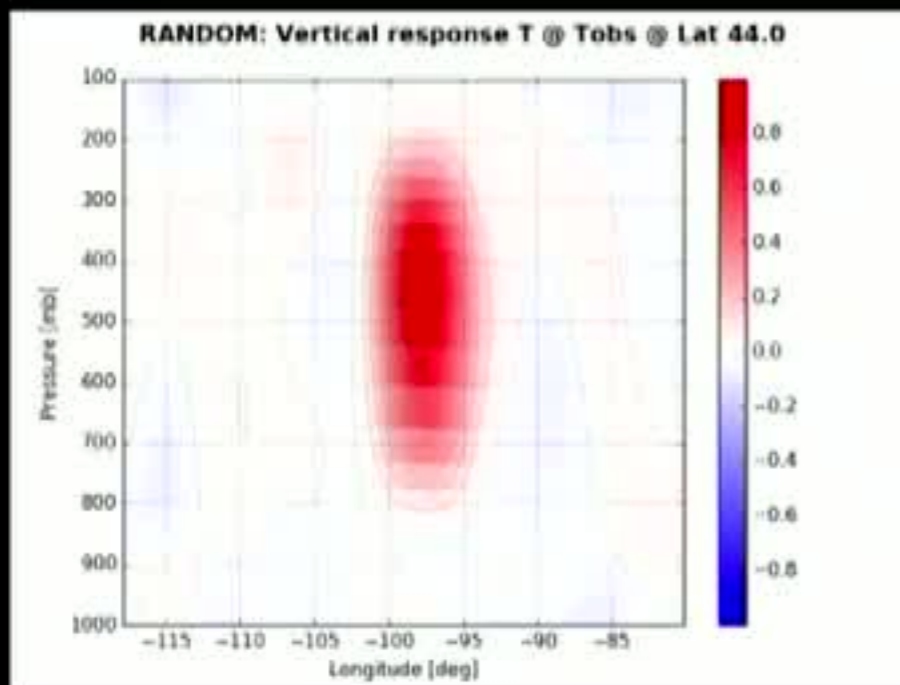
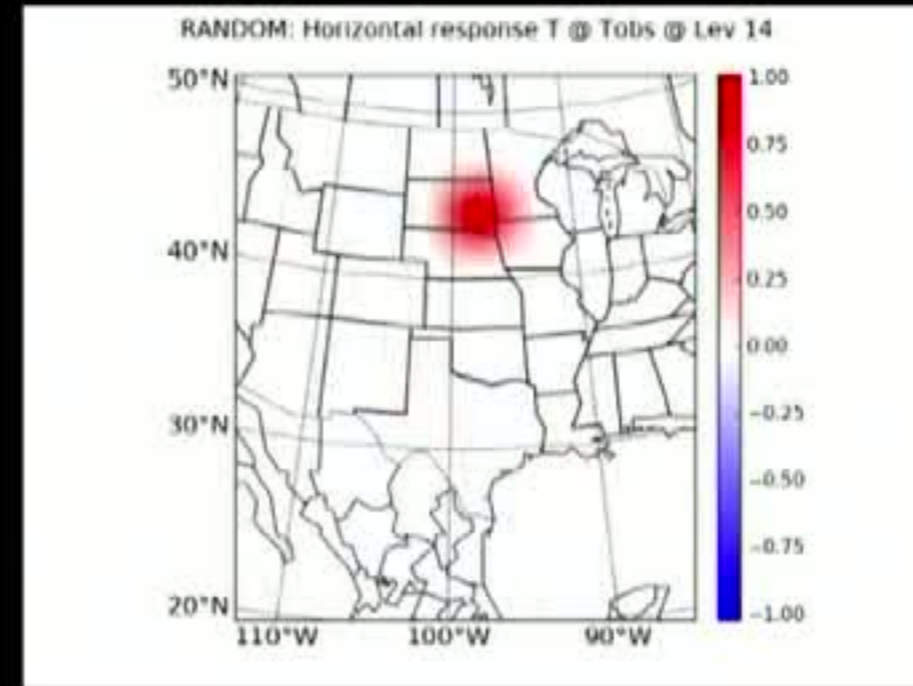
$$x^a - x^f = (L \circ P_E)^{1/2} (L \circ P_E)^{T/2} \frac{\Delta x}{(\sigma_f^2 + \sigma_R^2)} (0 \quad \dots \quad 1_k \quad \dots \quad 0)^T$$

Random autocovariance (COV_{T-T})

1024 ensembles



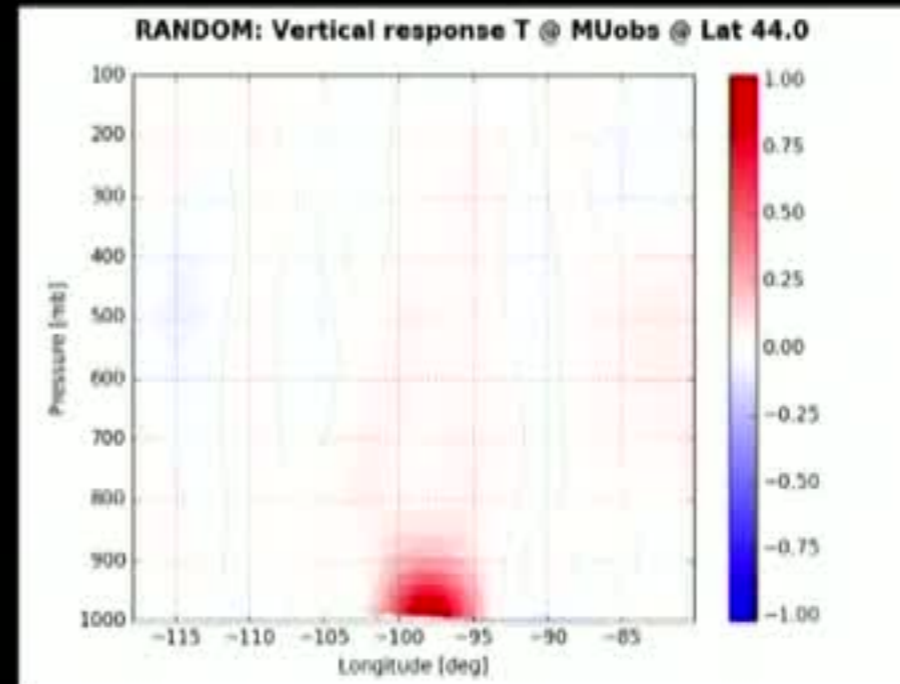
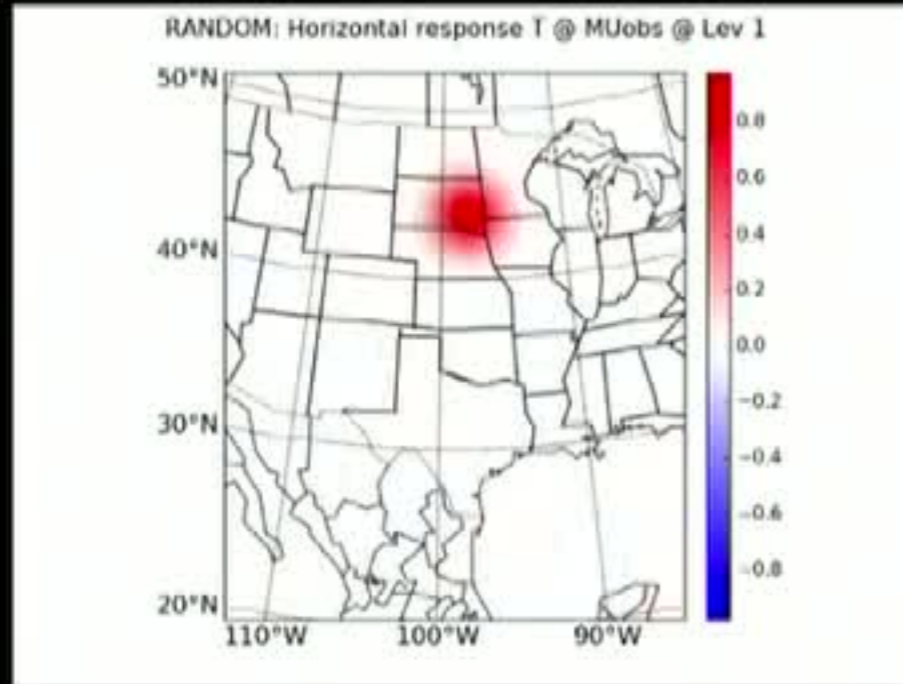
4096 ensembles



More random ensembles produce less noise

Results: random cross-covariance ($\text{COV}_{\text{PS-T}}$)

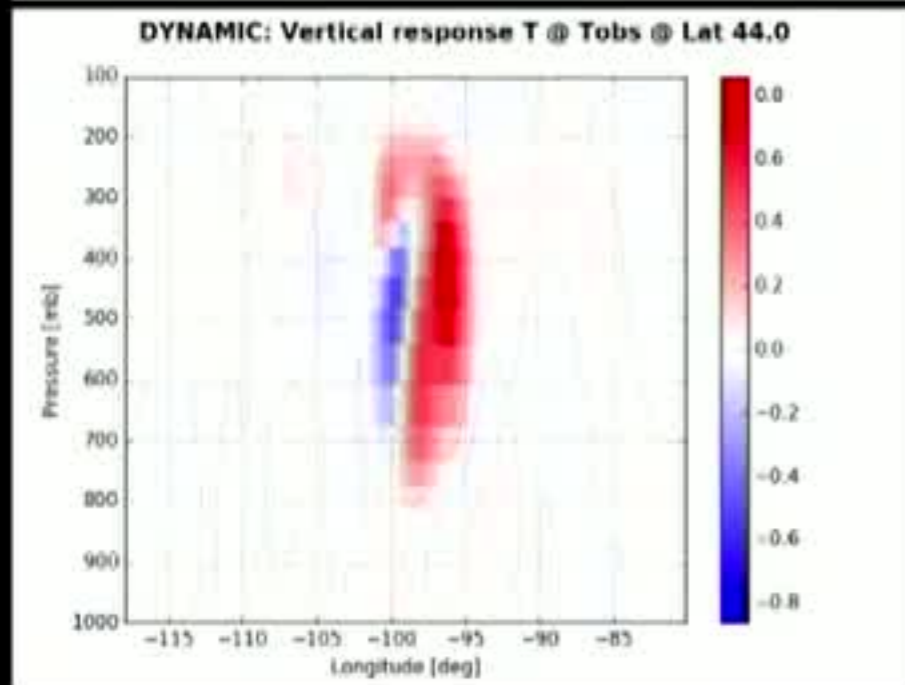
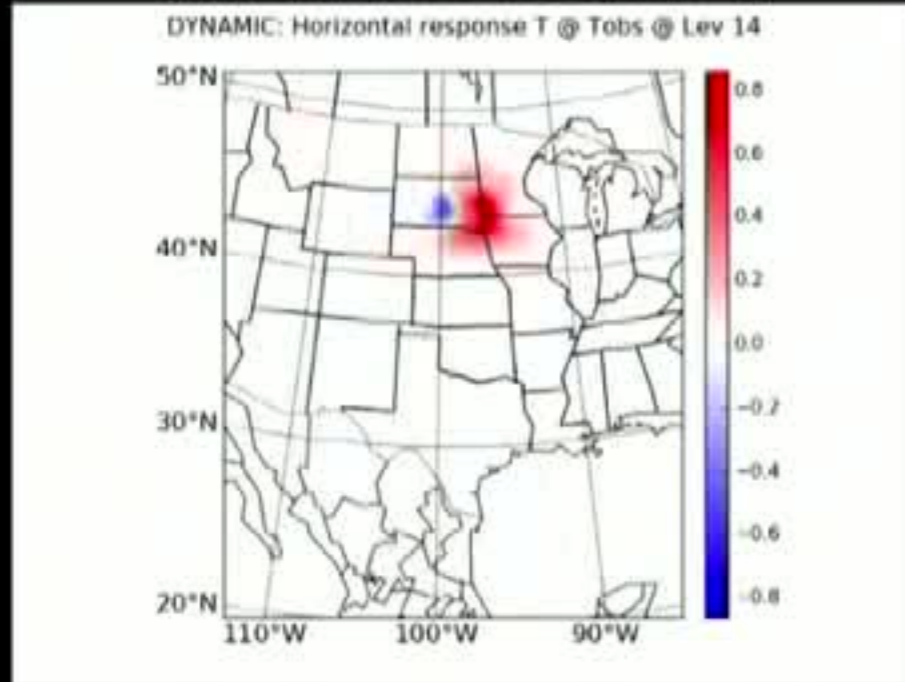
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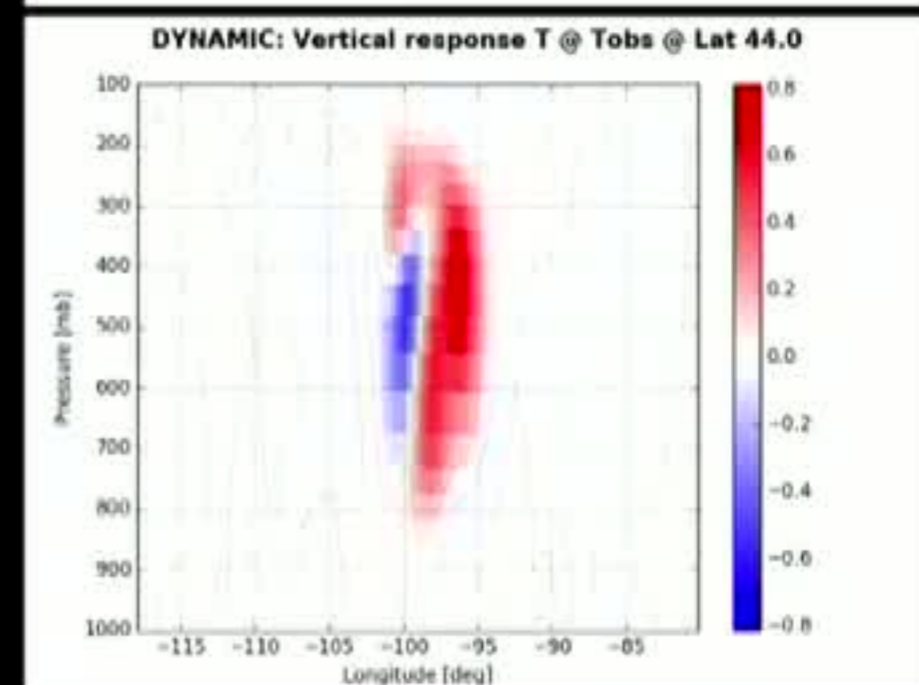
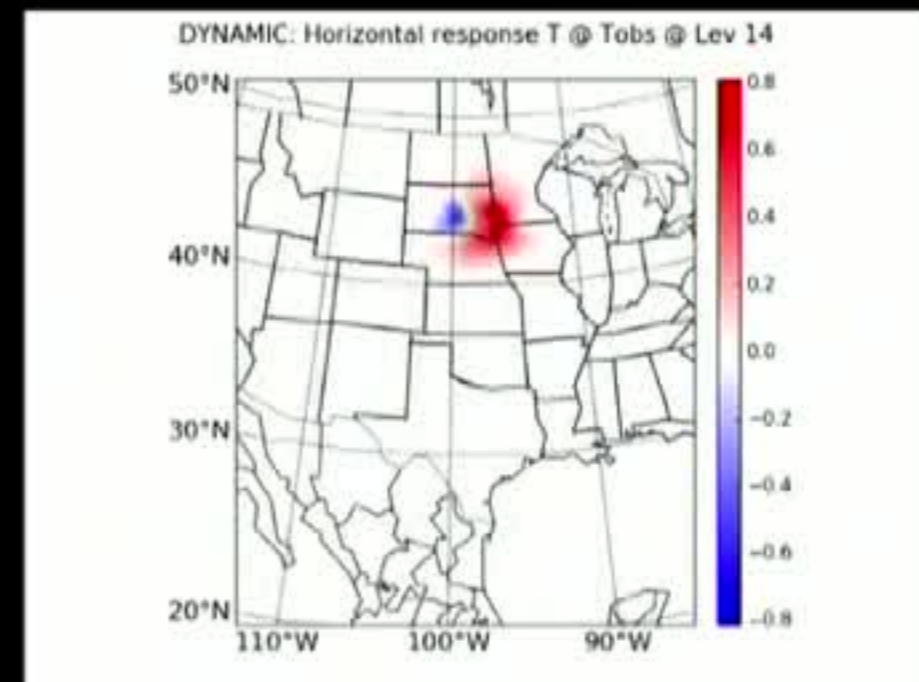
Acceptable noise in cross-covariances

Results: total autocovariance - COV_{TT} (4096 random x 32 dynamic)

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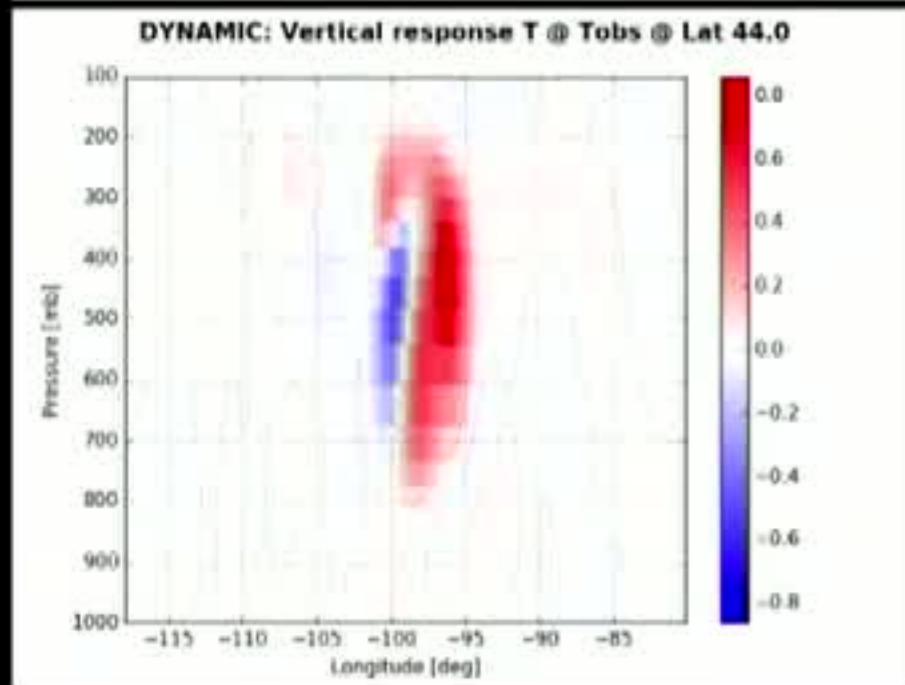
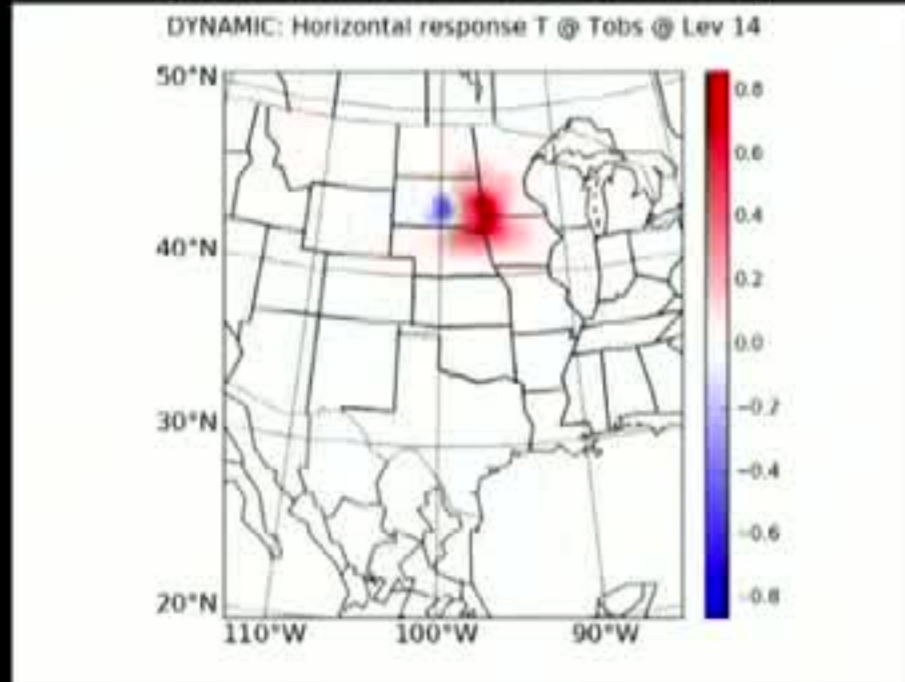


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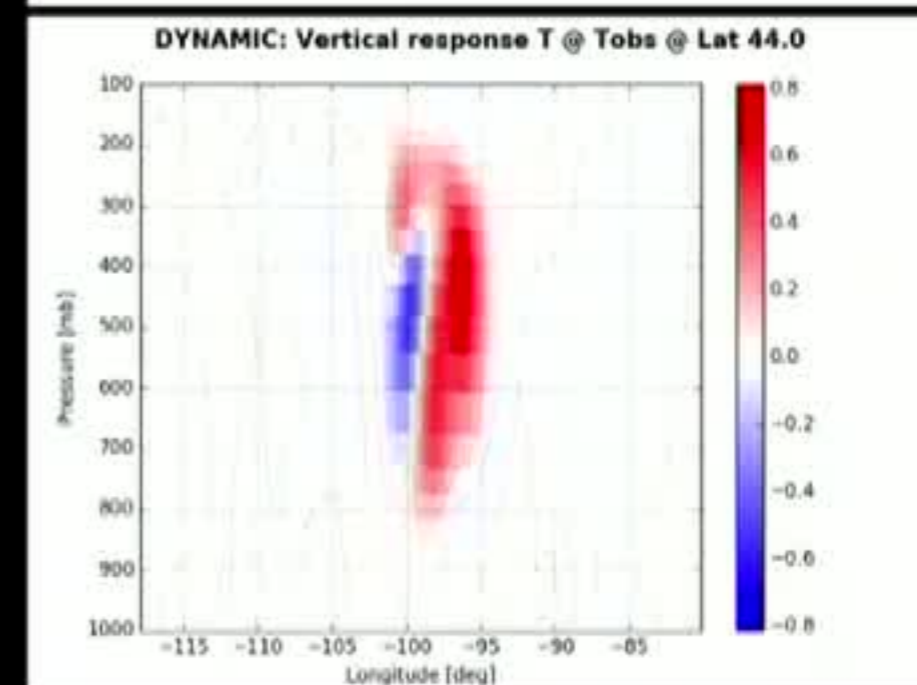
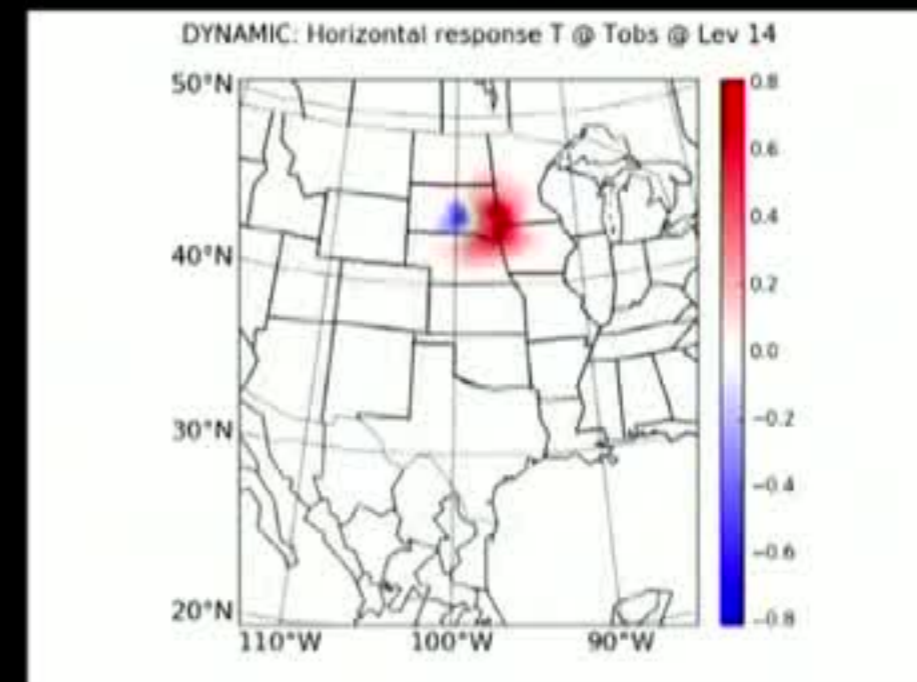


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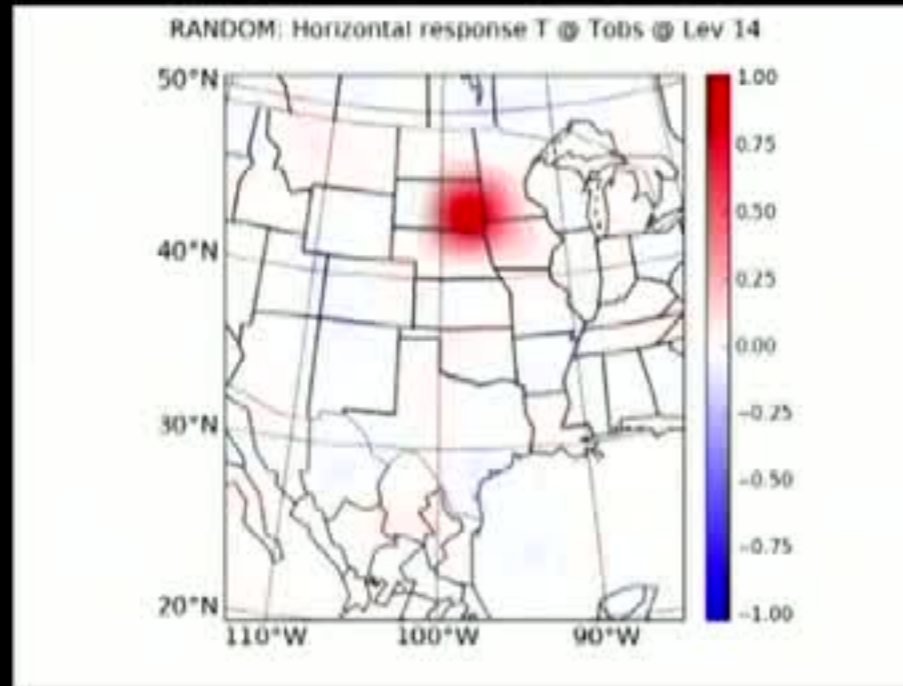


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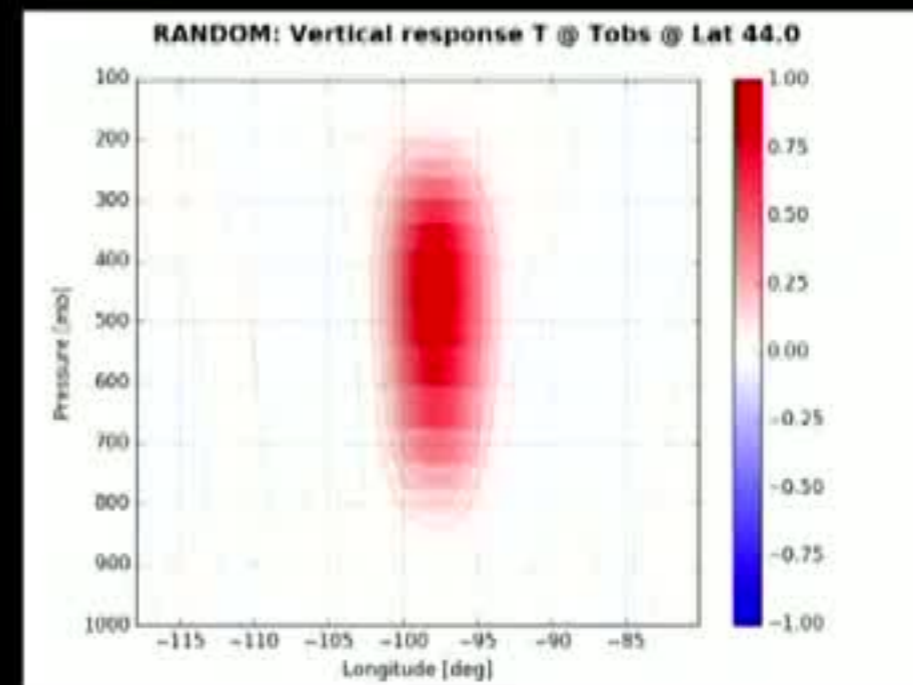
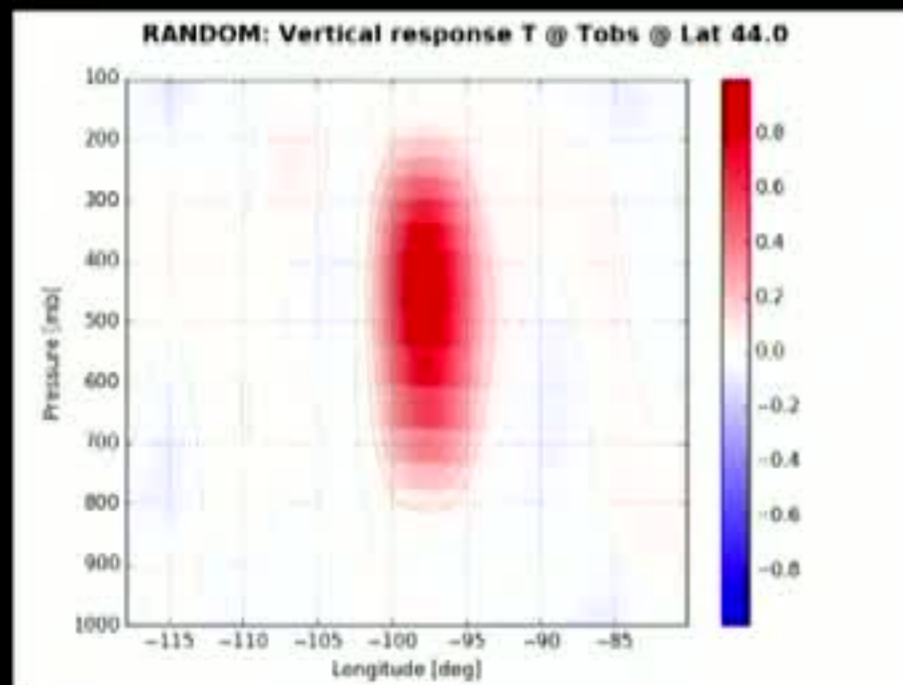
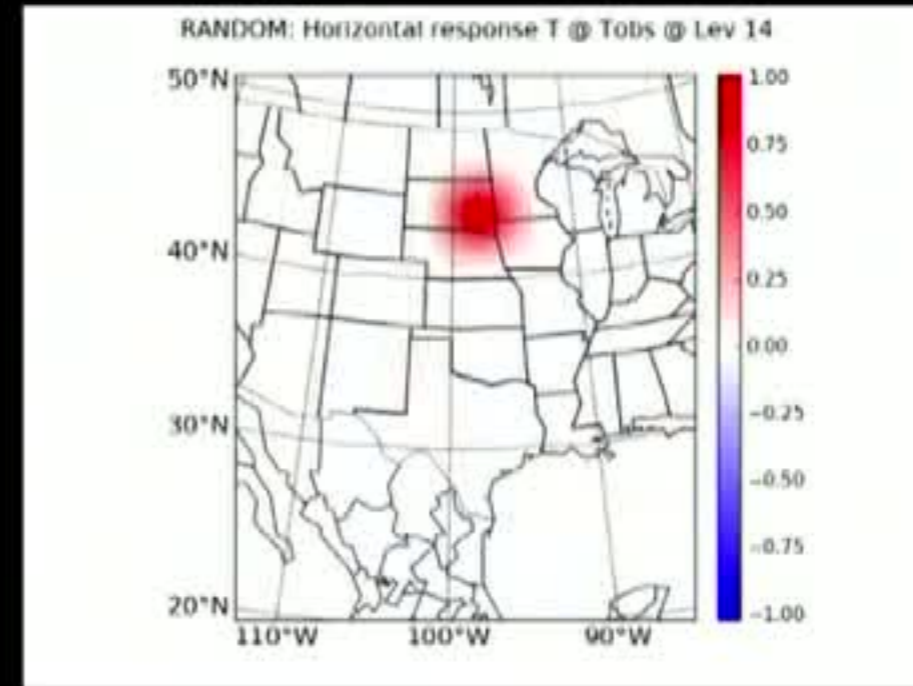


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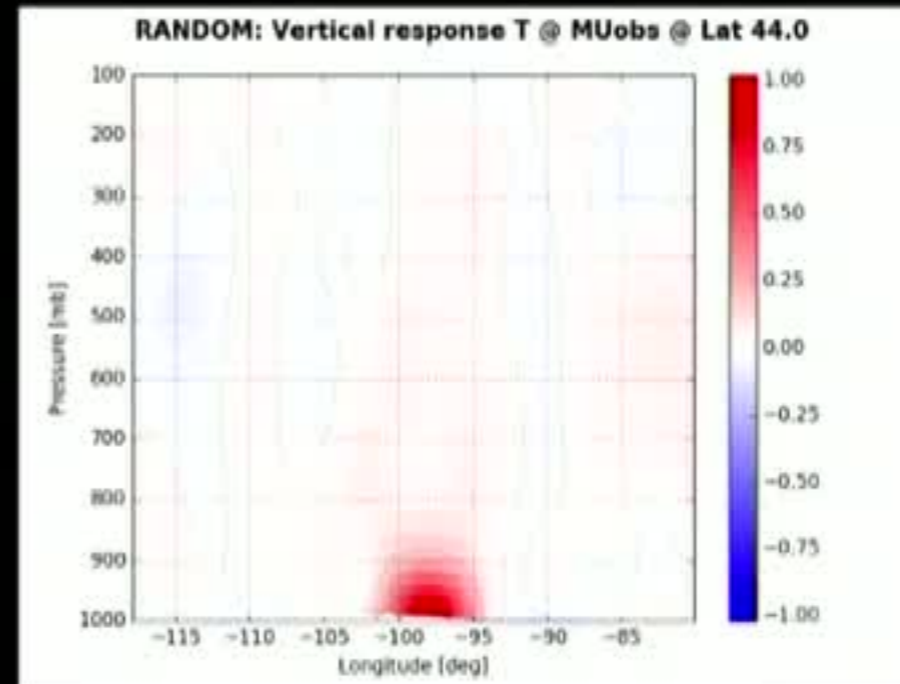
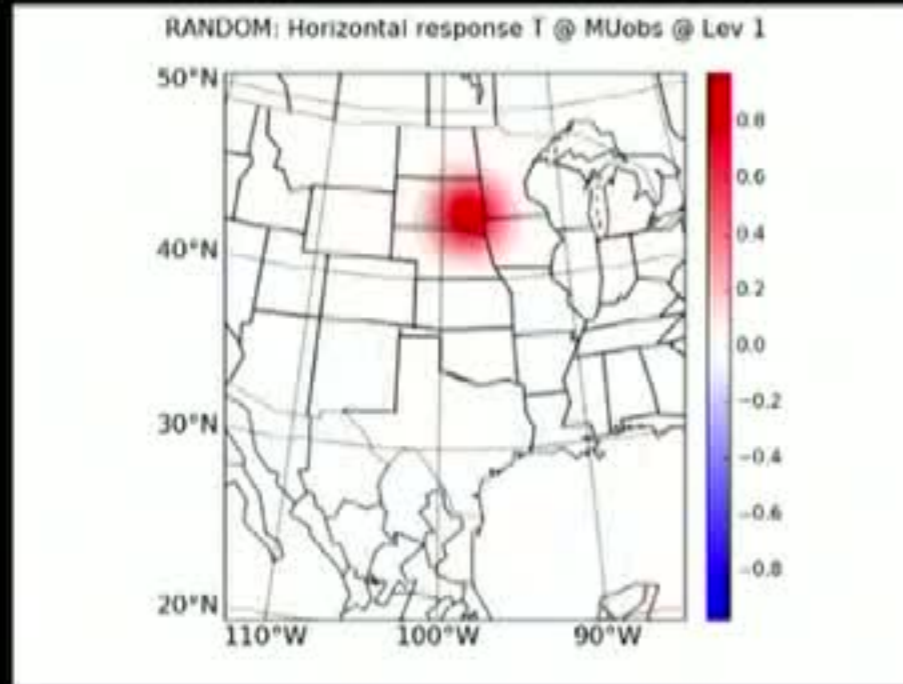
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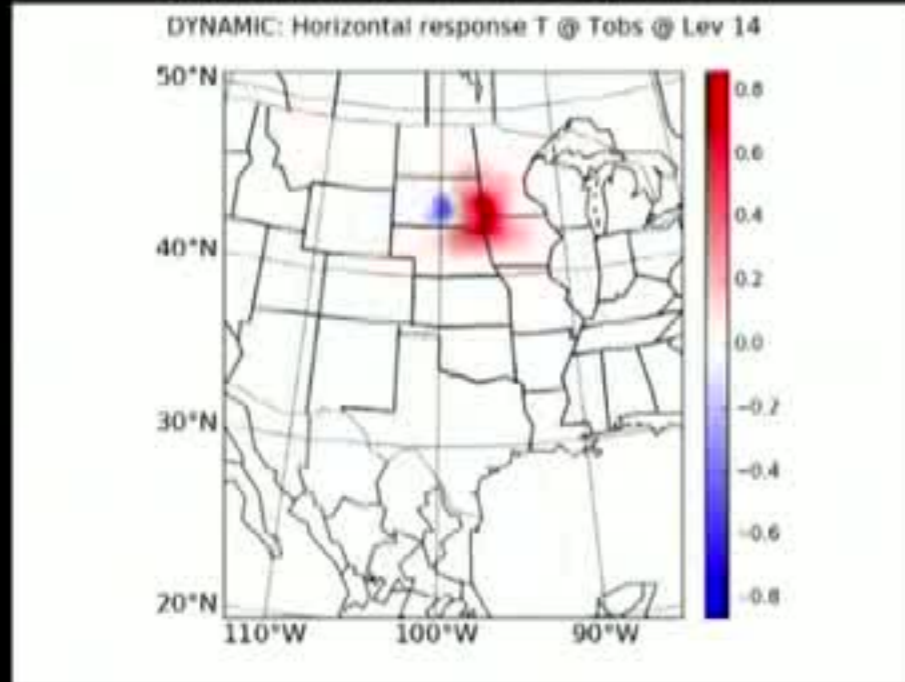
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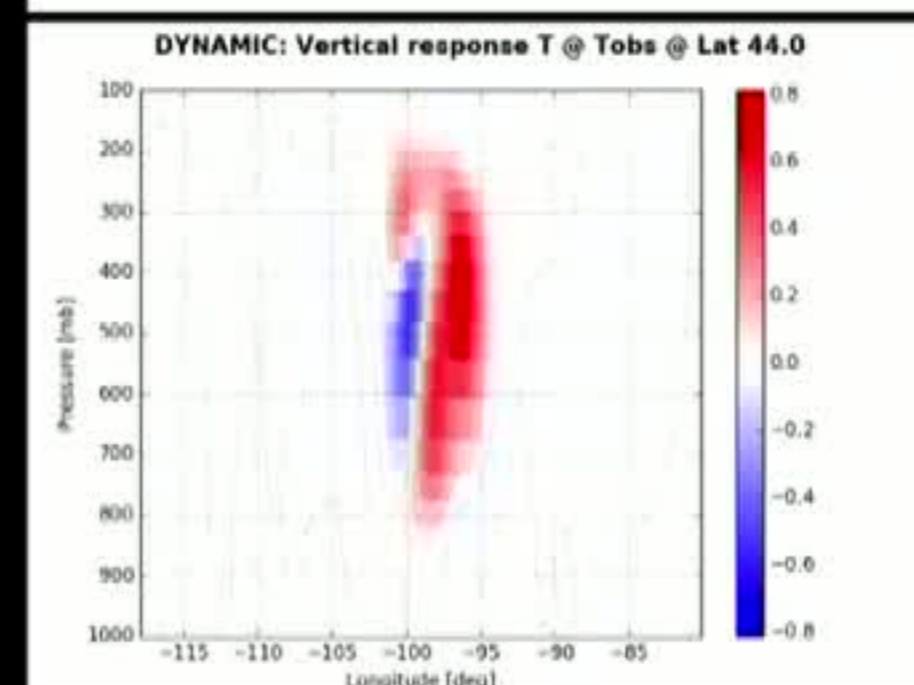
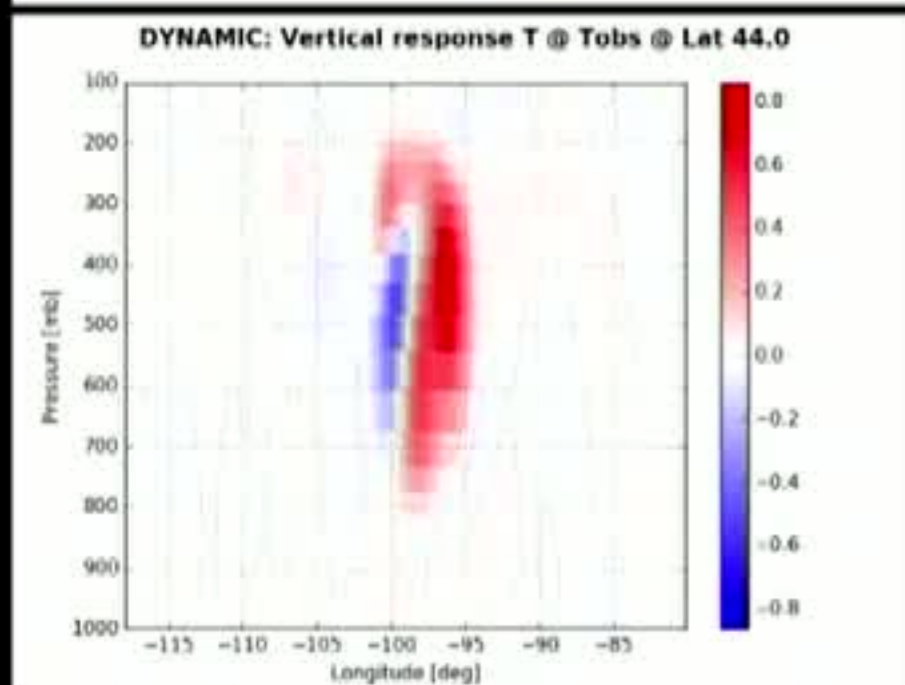
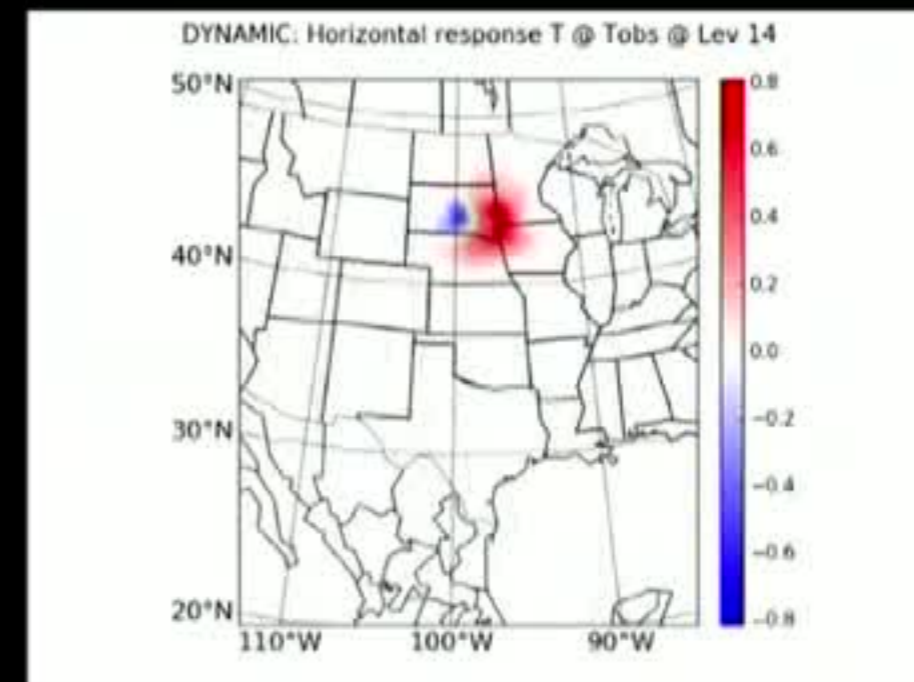
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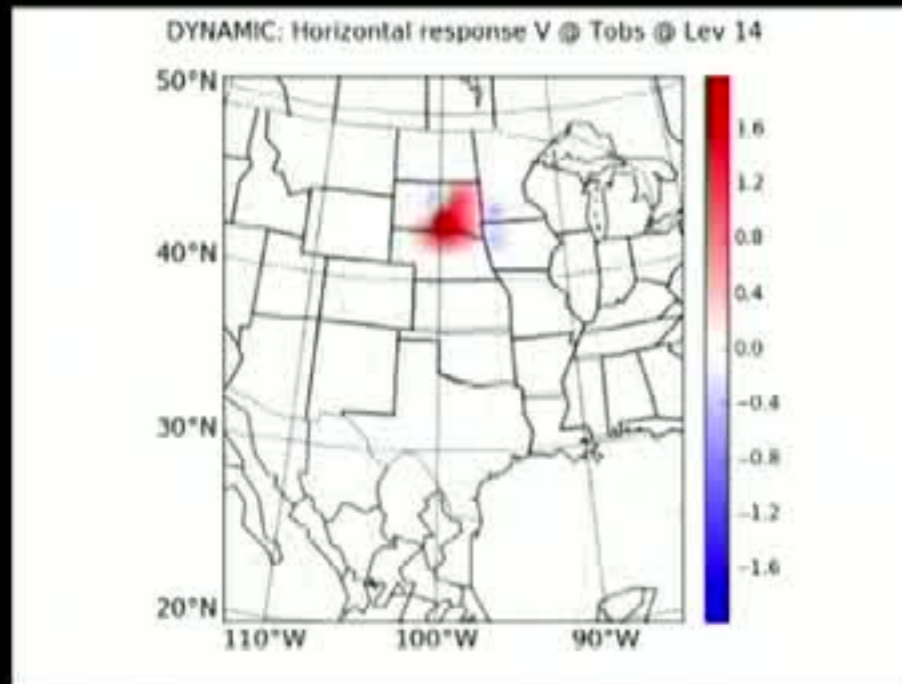


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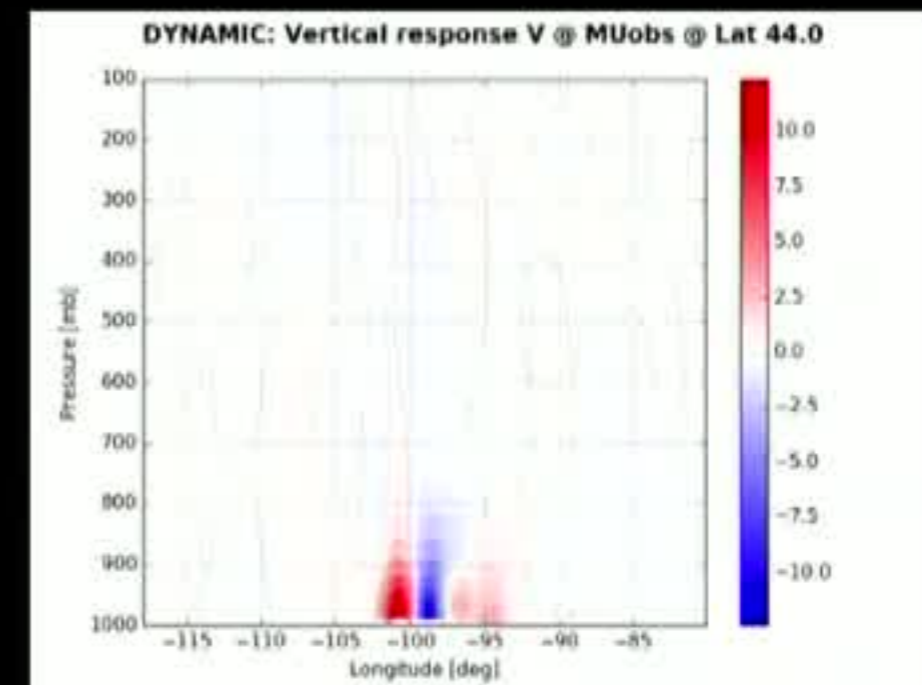
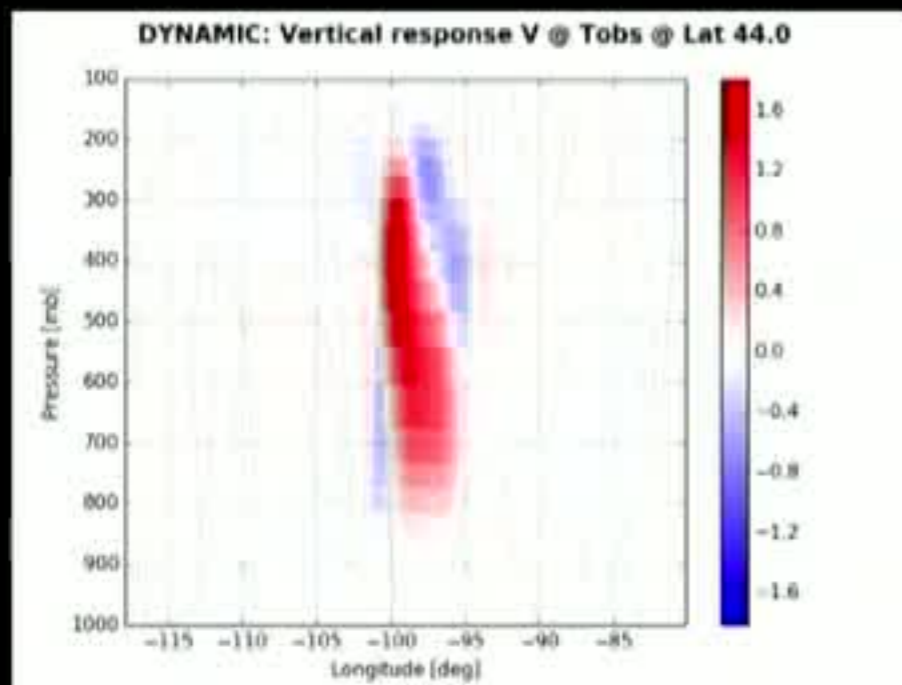
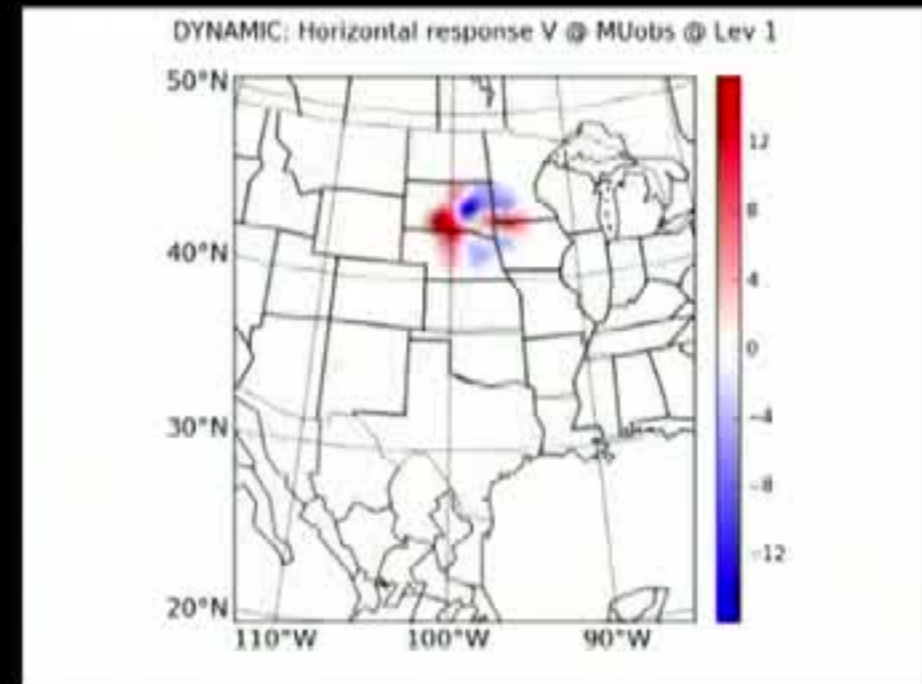


Results: total cross-covariance (4096 random x 32 dynamic)

$T_{\text{obs}} - V$ response



$MU_{\text{obs}} - V$ response



Complex structure a consequence of dynamical covariance

Practical considerations

- *Hadamard product is expensive to calculate*
 - Localized random vectors are calculated off-line $g_j = L^{1/2} \varphi_j, (j = 1, N_r)$
 - Calculation depends on state vector specification
- *Analysis space dimension is large (random x dynamic)*
 - Number of random ensembles does not depend on state dimensions (identity random matrix only)
 - need parallel programs to process $\sim O(10^5)$ ensembles
 - optional reduced Hessian preconditioning for even faster code
- *Need only 32 + 1024 files to produce 32 x 1024 columns of covariance*
 - high efficiency
 - possibility to introduce another orthogonal basis and substitute random sample