On Hybrid Approaches to Data Assimilation

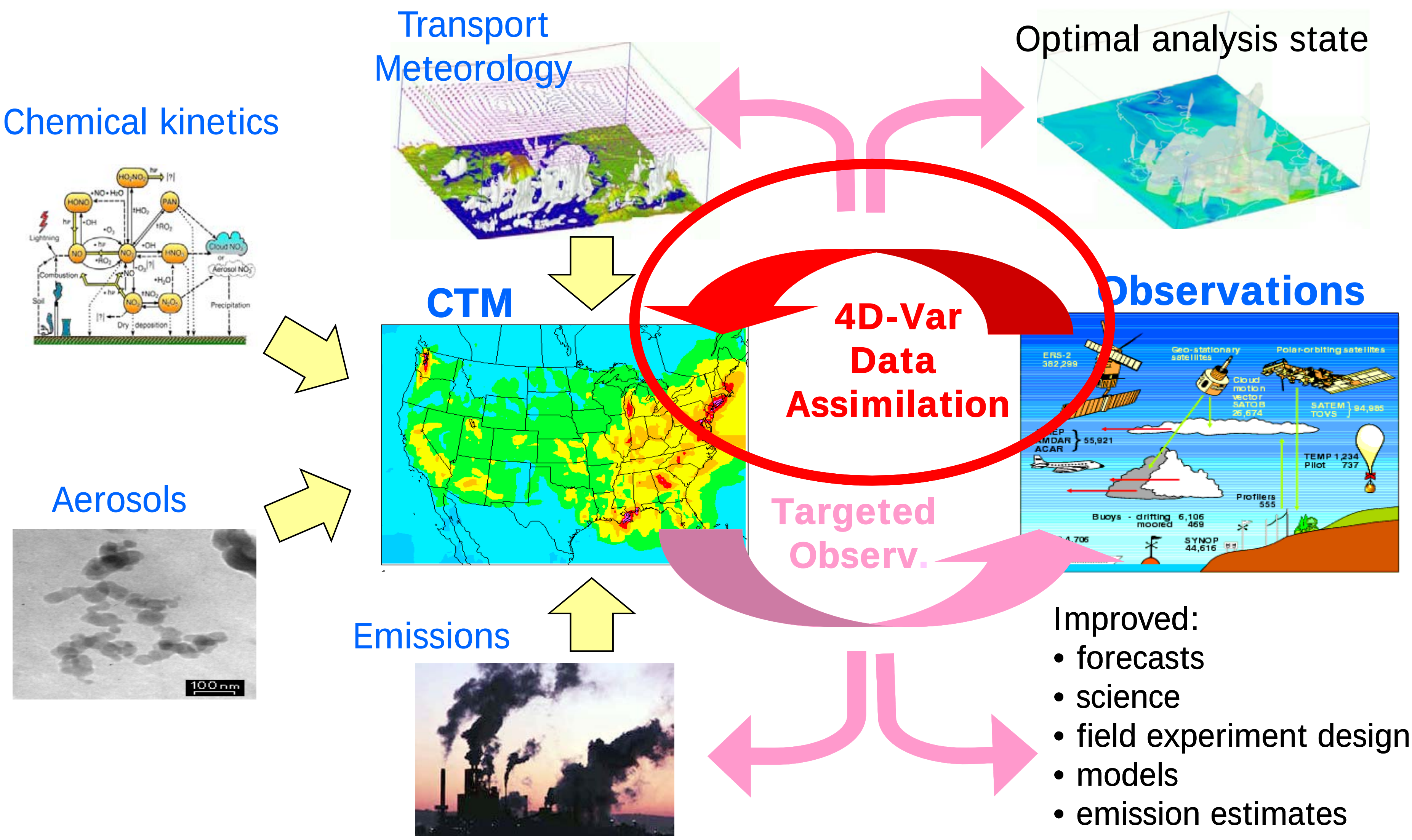
Adrian Sandu

Computational Science Laboratory

Computer Science Department

Virginia Tech

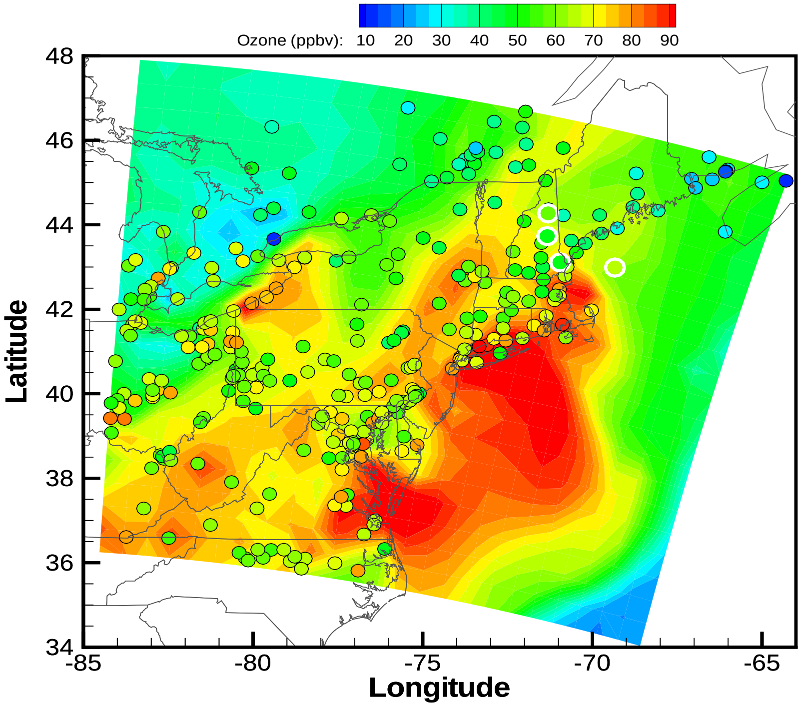
Information feedback loops between CTMs and observations: data assimilation and targeted meas.



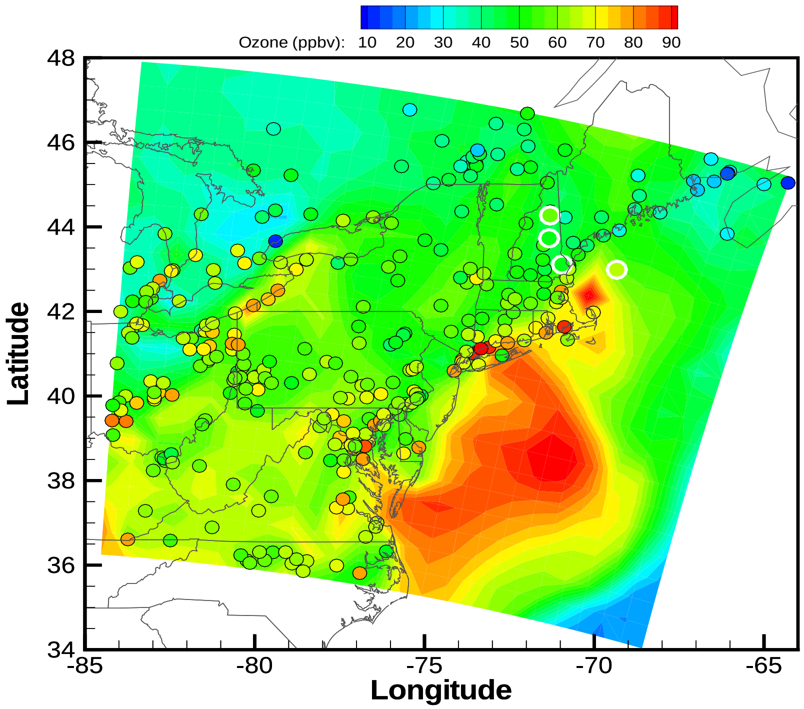
Assimilation adjusts O_3 predictions considerably at 4pm EDT on July 20, 2004

Observations: circles, color coded by O_3 mixing ratio

Surface O_3 (forecast)

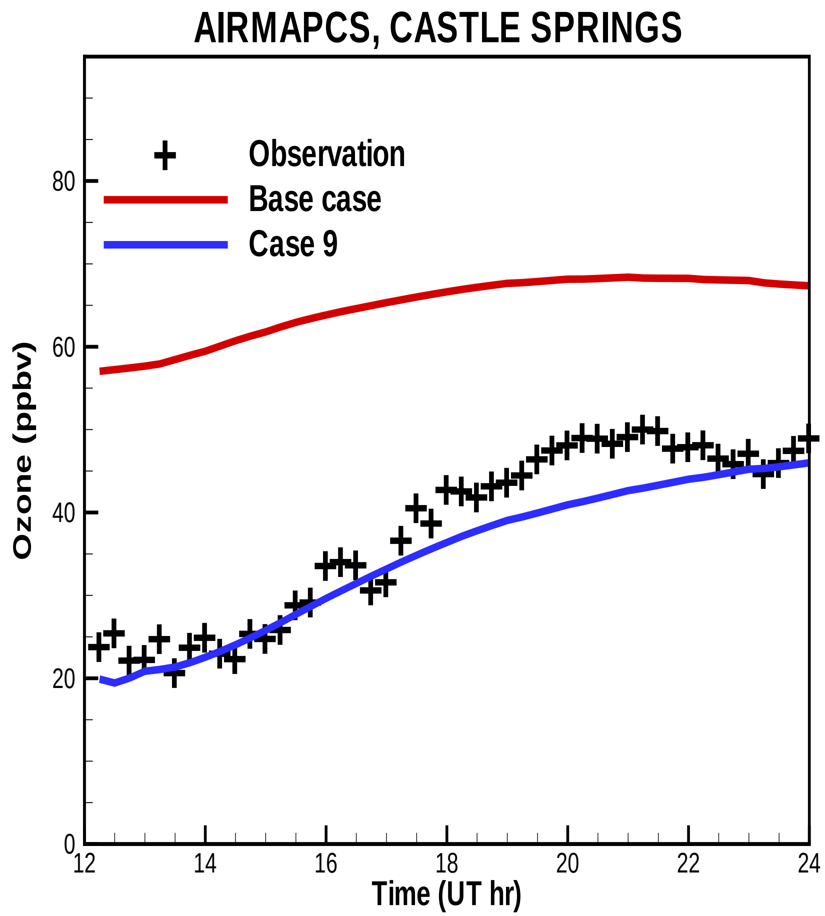


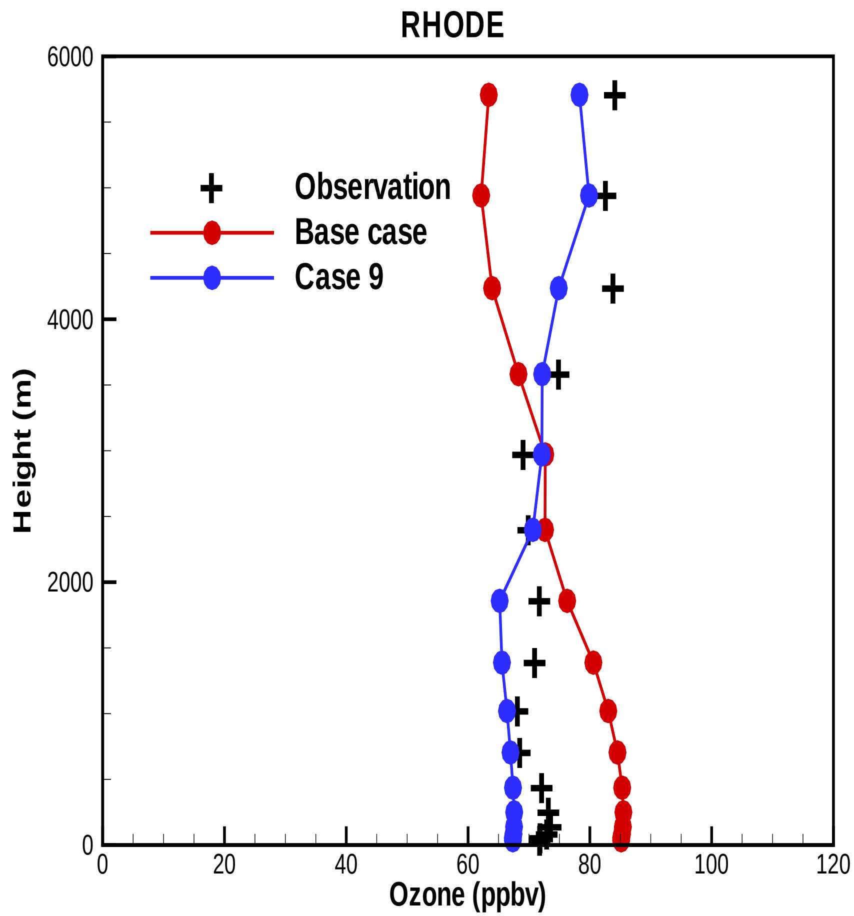
Surface O_3 (analysis)



[Chai et al., 2006]

Model predictions are in better agreement with observations after assimilation





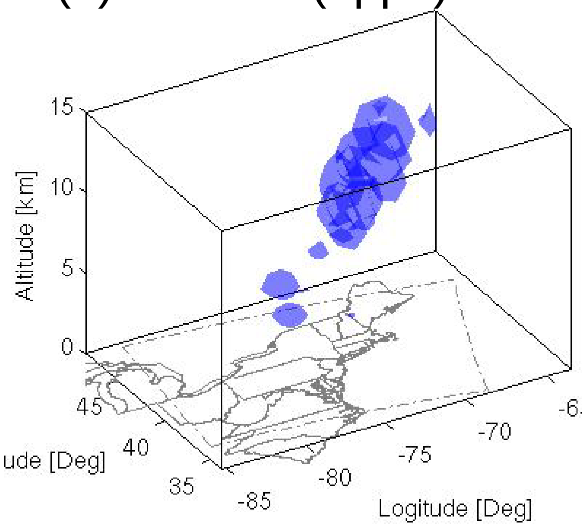
[Chai et al., 2006]

The smallest Hessian eigenvalues (vectors) approximate the principal error components

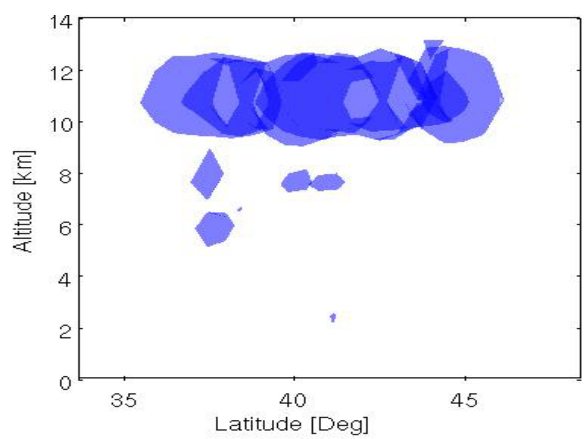
$$\left(\nabla^2_{y^0,y^0}\Psi\right)^{-1} \approx \mathrm{cov}\left(y^0\right)$$

	First	Second	Third	Fourth	Fifth
λ(H)	7.54e-25	1.15e-23	4.04e-23	8.47e-23	1.42e-22
λ(P)	1.33e+24	8.70e+22	2.48e+22	1.18e+22	7.04e+21
STD (ppb)	47	3	0.87	0.41	0.25

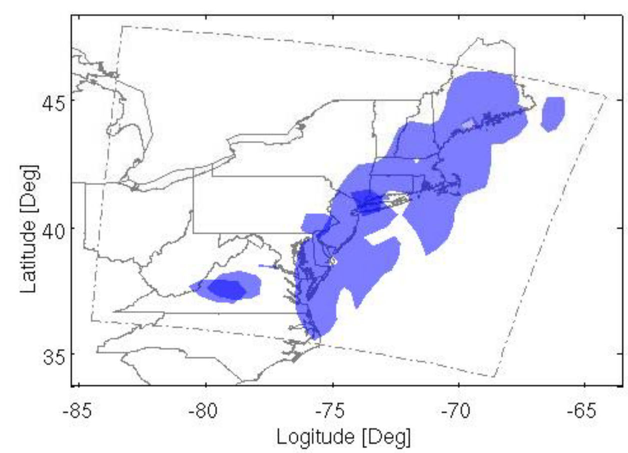
(a) 3D view (5ppb)



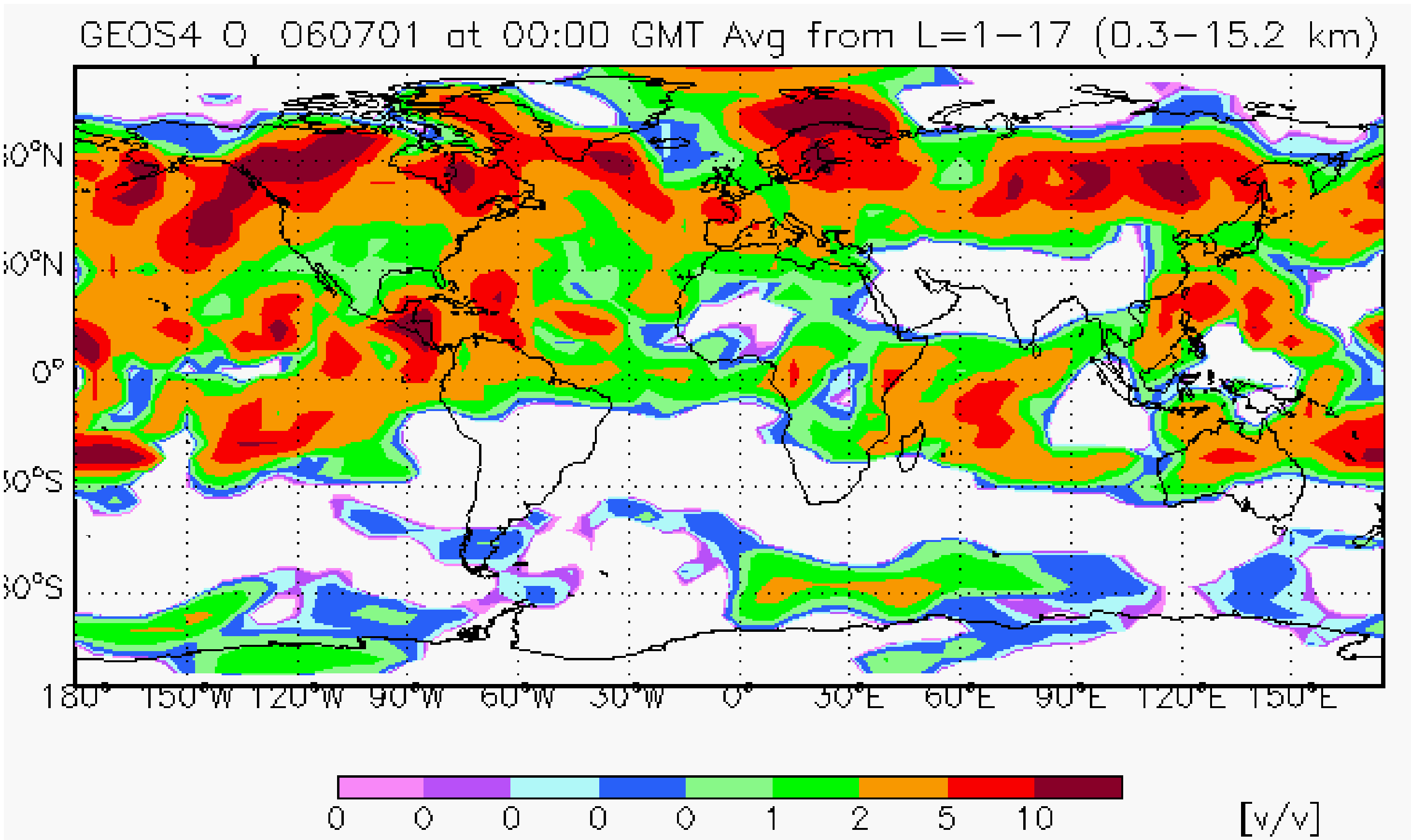
(b) East view



(c) Top view

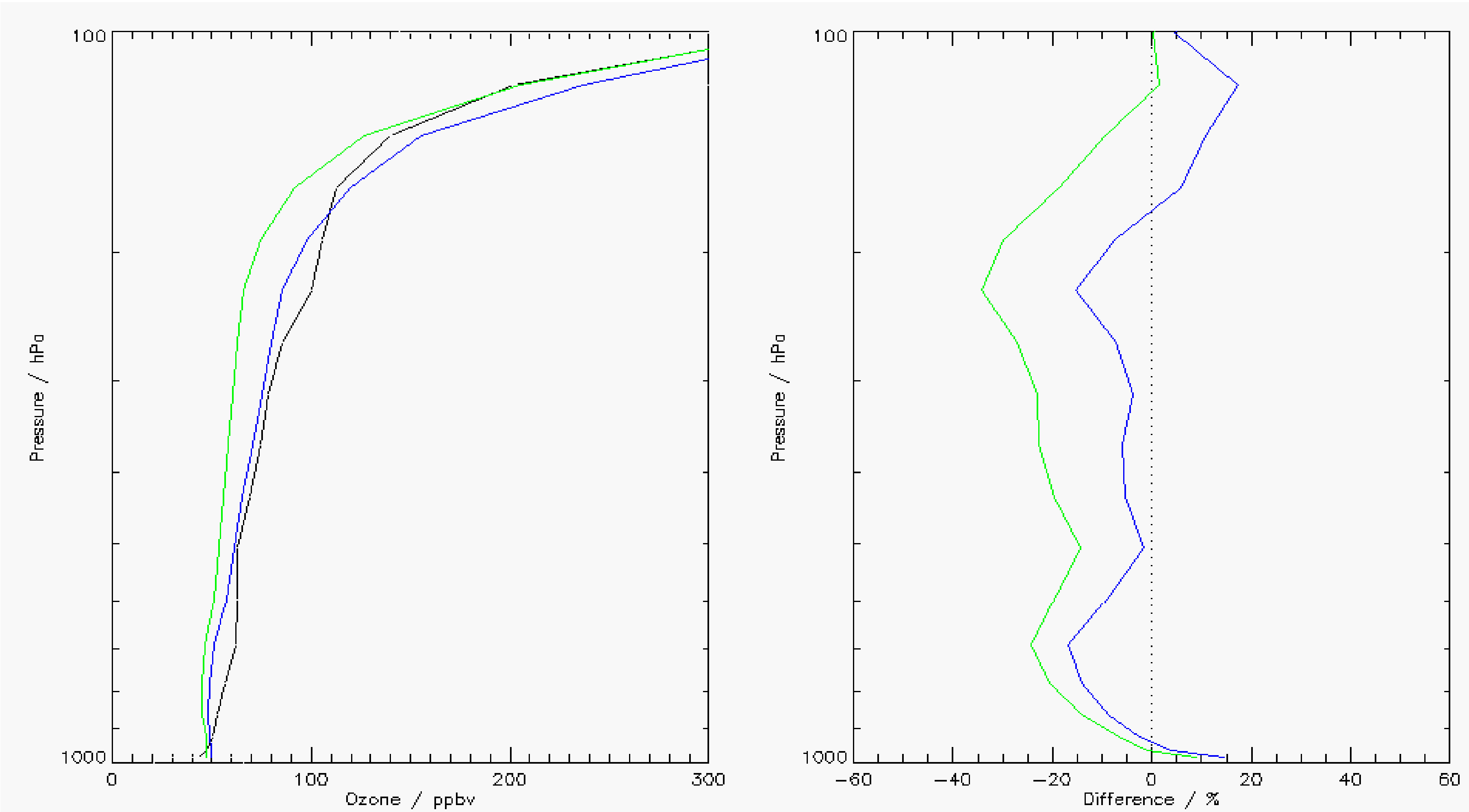


4D-Var Data Assimilation of TES (Satellite) Ozone Profile Retrievals with GEOS-Chem

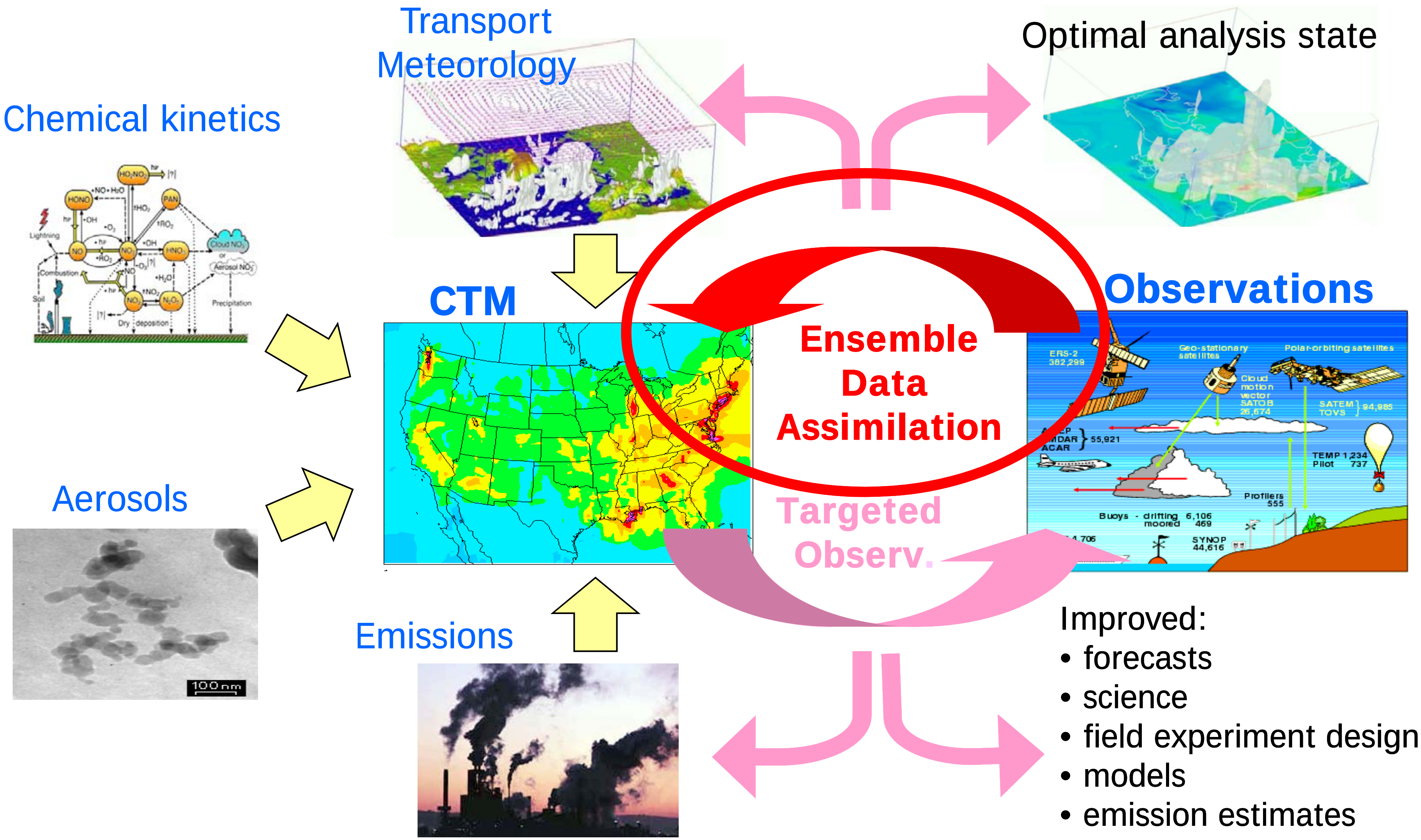


Plots from difference between background ozone field and analysis ozone field through TES profile retrievals for 2006 summertime GEOS-Chem data

Validation of GEOS-Chem Background and Analysis Against IONS Ozonesonde Profiles



Ensemble-based chemical data assimilation can complement variational techniques



Covariance inflation and localization are necessary to compensate for small ensemble size

Covariance inflation:

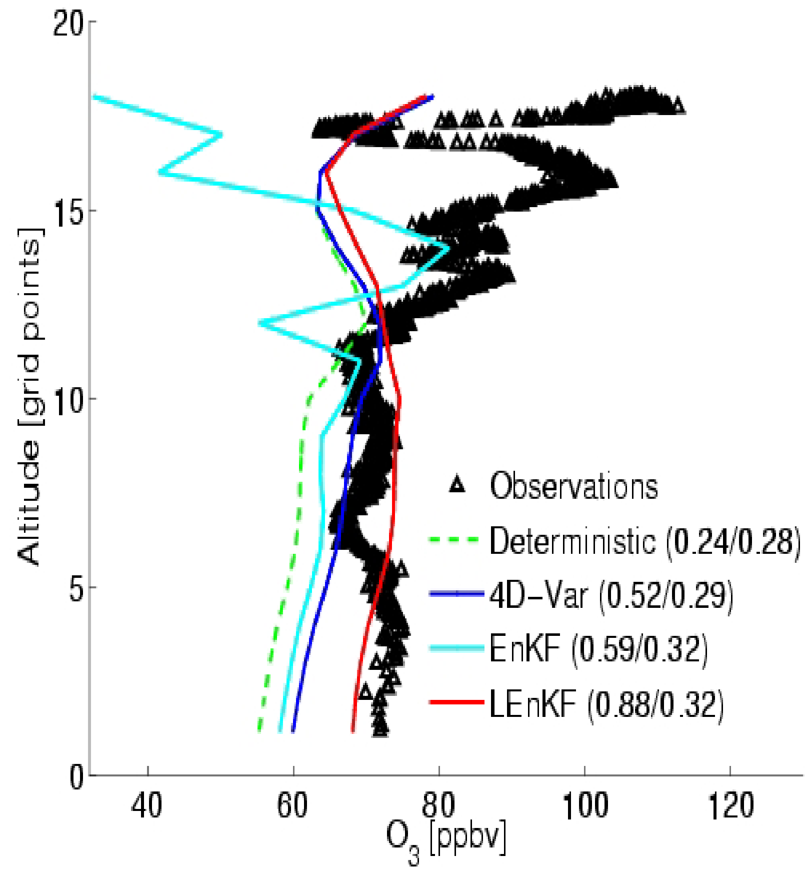
- Prevents filter divergence
- Additive
- Multiplicative
- Model-specific

Covariance localization:

- Limit long-distance correlations according to NMC empirical ones

Correction localization:

- Limit increments away from observations

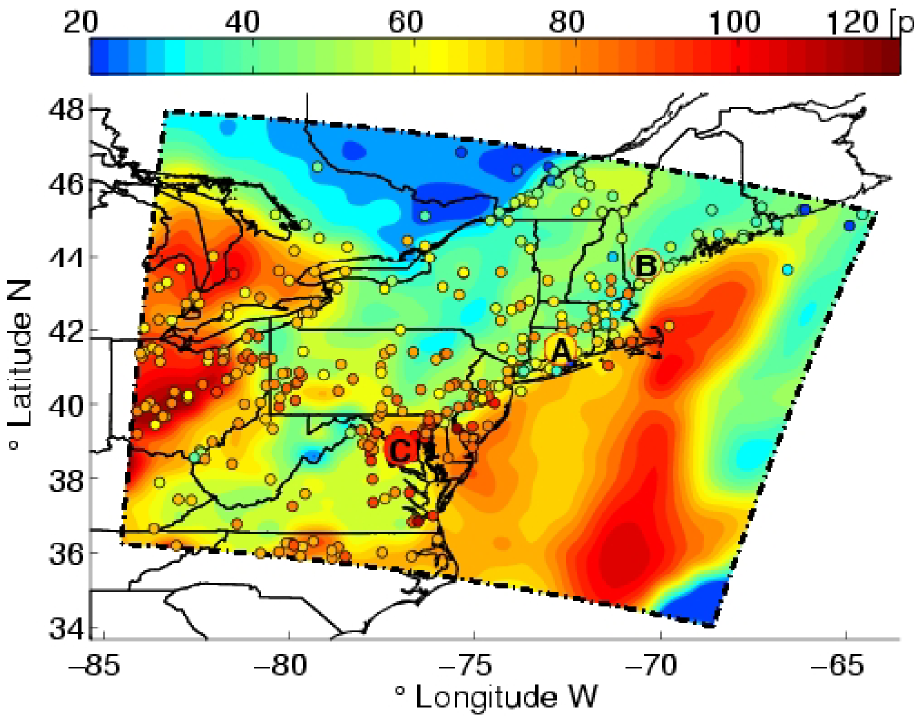


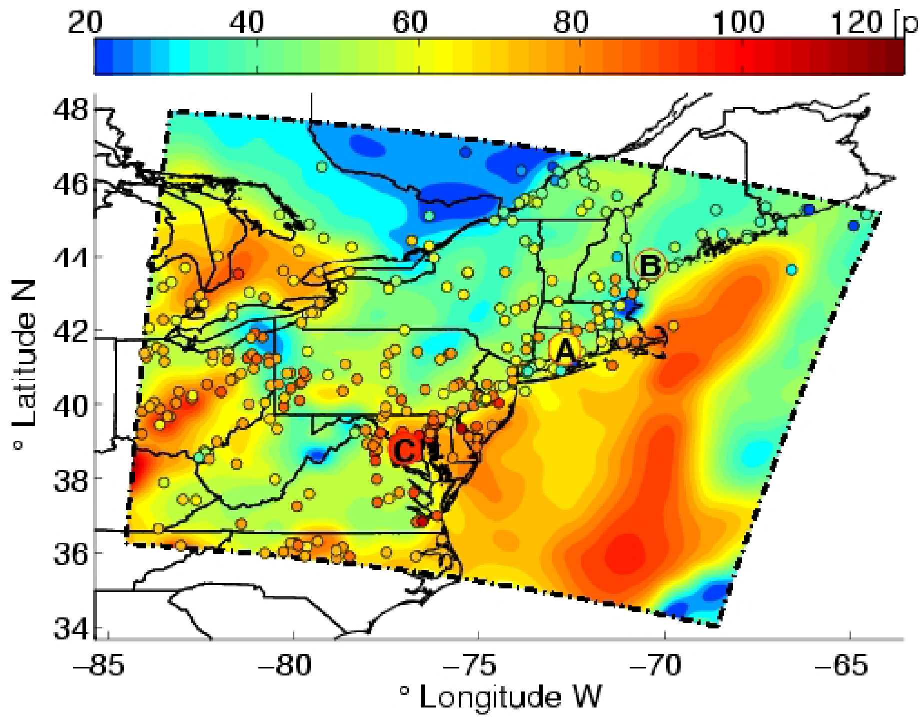
Ozonesonde S2 (18 EDT, July 20, 2004)

LEnKF assimilation of emissions and boundaries together with the state can improve the forecast

Ground level ozone at 14 EDT, July 21, 2004 (in forecast window)

LEnKF (R^2=0.88/0.32) [state only] | LEnKF (R^2=0.88/0.42) [state + emissions + boundary]





4D-Var Features

Pros:

- considers all observations within one assimilation window at the same time
- generates analysis that is consistent with the system dynamics

Cons:

- assumes constant background covariance matrix at the beginning of each assimilation window
- requires building the adjoint model

EnKF Features

Pros:

- simple concept, easy implementation
- updates system states and covariance
- no adjoint model required

Cons:

- non-smooth analysis state flow
- sampling error is large in large-scale models

Questions

- Can we better understand the relationship between variational and ensemble based methods for data assimilation?
- Can we use this understanding to build hybrid assimilation methods that combine the strengths of both approaches?

Hybrid Approach for Error Covariance Update

- Problem: The background error covariance matrix is kept constant between 4D-Var assimilation windows.
- Solution: Update the error covariance matrix at the end of each assimilation window.
- Procedure:
    - Explore the 4D-Var error reduction directions.
    - Generate a space spanned by the error reduction.
    - Project the ensemble background perturbation on the orthogonal complement of the space.
- The background ensemble runs can be performed in parallel with 4D-Var without incurring a significant computational overhead.

Background Ensemble Generation

- Generate a set of *Nens* normally distributed perturbations with mean zero and covariance B_{t_0}:

$$\Delta x_i^b(t_0) \in \mathcal{N}(0, B_{t_0}) \ , \quad i = 1, \ldots Nens \ .$$

- Construct a background ensemble of size *Nens*:

$$x_i^b(t_0) = x^b(t_0) + \Delta x_i^b \ , \quad i = 1, \ldots, Nens \ .$$

- Propagate this ensemble to the end of the assimilation window.

$$x_i^b(t_1) = \mathcal{M}_{t_0 \to t_F}\left(x_i^b(t_0)\right) \ , \quad i = 1, \ldots, N_{ens}$$

- Compute the mean $x^b(t_1)$ and background ensemble perturbation:

$$\Delta x_i^b(t_1) = x_i^b(t_1) - x^b(t_1)$$

Subspace of Error Reduction

- 4D-Var optimization generates iterates

$$x_0^{(j)}\ ; \quad x_1^{(j)} = \mathcal{M}_{t_0 \to t_1}\,(x_0^{(j)}), \quad j = 1, \dots k.$$

- The space spanned by the normalized 4D-Var increments

$$\mathcal{S}_{t_1} = \left[\frac{x_1^{(j)} - x_1^{(j-1)}}{\left\| x_1^{(j)} - x_1^{(j-1)} \right\|} \right]_{j=1,\dots,k} \approx \text{span}\left\{ U_{t_1} \right\}$$

- Orthogonal projector onto the orthogonal complement of U_{t_1}:

$$\mathcal{P}_{t_1} \;\; = \;\; I - U_{t_1} U_{t_1}^T$$

Hybrid Ensemble Generation

- Projected ensemble:

$$\Delta x_i^p(t_1) \;=\; \mathcal{P}_{t_1} \Delta x_i^b(t_1)$$

- Karhunen-Loève decomposition of approximate Hessian inverse leads to approximate analysis perturbation:

$$H^{-1} = \sum_{j=1}^{d} \lambda_j w_i w_j^T \,, \quad \Delta x_i^{Hess} = \sum_{j=1}^{d} \xi_j^i \sqrt{\lambda_j} w_j, \quad \xi_j^i \in \mathcal{N}(0,1).$$

- Hybrid ensemble:

$$\Delta x_i^h(t_F) = \Delta x_i^p(t_F) + \Delta x_i^{Hess}(t_F).$$

Hybrid Covariance Matrix

- Compute hybrid ensemble covariance matrix:

$$\widehat{B}^h_{t_F} = \frac{\left(\Delta x^h_i\right) \cdot \left(\Delta x^h_i\right)^T}{\sqrt{Nens - 1}}.$$

- Localize hybrid ensemble covariance matrix:

$$B^h_{t_F} = \rho \otimes \widehat{B}^h_{t_F}$$

- Updated background covariance through a convex combination of the static background covariance B_0 and the hybrid covariance $B^h_{t_F}$ as:

$$A_{t_F} = \alpha \cdot B_0 + (1 - \alpha) \cdot B^h_{t_F} \ ,$$

Numerical Tests on Lorenz 96 Model

$$\frac{dx_j}{dt} = -x_{j-1}(x_{j-2} - x_{j+1} - x_j) + F \ , \ \ j = 1, \dots 40 \ ,$$

periodic boundary conditions, $F = 8.0$.
The background covariance B_{t_0} is constructed from a 3% perturbation of the initial state, and a correlation distance of $L = 1.5$:

$$B_{t_0}(i,j) = \sigma_i \cdot \sigma_j \cdot \exp\left(-\frac{|i-j|^2}{L^2}\right) \ , \ \ i, j = 1, \dots, 40 \ .$$

The observation covariance matrix is diagonal from a $\rho = 1\%$ perturbation from the mean observation values. The observation operator $\mathcal{H}$ captures only a subset of 30 model states, which includes every other state from the first 20 states plus the last 20 states.

Analysis RMS Error Comparison

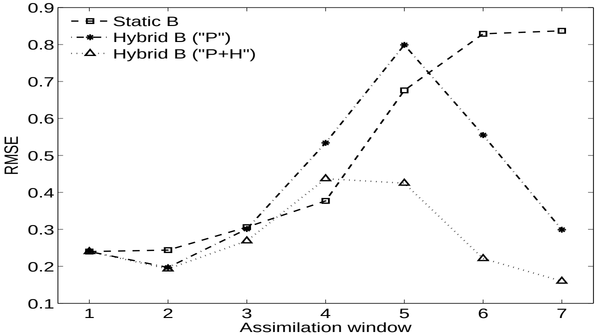


Figure: Analysis RMSE comparison for seven assimilation windows, using different background covariance matrices (static and hybrid covariances with localization length $L = 5$, and blending factor $\alpha = 0.2$; P is projection only, P+H is projection with Hessian enhancement).

How Similar are 4D-Var and EnKF? Analysis Assumptions

For $x_0 \in \mathcal{N}\left(\mathbf{x}_0^B, \mathbb{B}_0\right)$. A linear, invertible model solution operator $\mathbf{M}$ advances the state from t_0 to t_F,

$$\mathbf{x}(t_F) = \mathbf{M} \cdot \mathbf{x}(t_0) \ .$$

The mean background state and the background covariance at t_F are

$$\mathbf{x}_F^B = \mathbf{M} \cdot x_0^B \ , \quad \mathbb{B}_F = \mathbf{M} \cdot \mathbb{B}_0 \cdot \mathbf{M}^T \ .$$

A set of noisy measurements taken at t_F (a single 4D-Var assimilation window).

$$\mathbf{y}_F = H \cdot \mathbf{x}_F + \varepsilon_F \ , \quad \varepsilon_F \in \mathcal{N}\left(0, \mathbb{R}_F\right).$$

How Similar are 4D-Var and EnKF? Analysis Result

Proposition:

If the model is linear and invertible; the errors are Gaussian; and observations are taken at a single time at the end of the assimilation window;

Then the numerical solution obtained by (imperfect, preconditioned) 4D-Var is equivalent to that obtained by the EnKF method with a small number of ensemble members.

The Analysis Motivates a Hybrid Approach

1. Run a short window 4D-Var, and perform $K+1$ iterations. The space spanned by the direction increments has an orthonormal basis
$$\widetilde{v}_1, \cdots, \widetilde{v}_K$$
2. Generate EnKF ensemble of K members. Replace the random sample from the normal distribution with K directions from the 4D-Var increment subspace (properly scaled).
3. Run EnKF for longer time.
4. Re-generate directions by another short window 4D-Var, and repeat.

Tests with the Nonlinear Lorenz Model

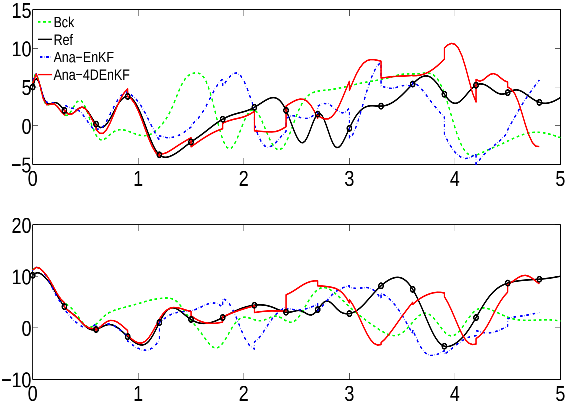


Figure: Solution comparison (with 10 ensemble members) for the first two components of the Lorenz state vector. Hybrid EnKF uses 4D-Var directions obtained from 0.2 time units.

Tests with the Nonlinear Lorenz Model

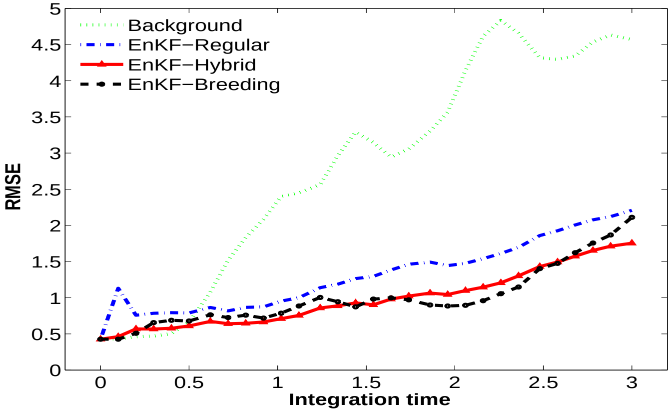


Figure: RMSE comparison for 10 ensemble members. Hybrid EnKF uses 4D-Var directions obtained from 0.2 time units. Errors shown are averages of 1000 runs.

Summary

- Can we better understand the relationship between variational and ensemble based methods for data assimilation?
- Can we use this understanding to build hybrid assimilation methods that combine the strengths of both approaches?
- Hybrid approach to improve background covariance
- Hybrid filter based on 4D-Var directions