



GSI Hybrid/4DEnVar Data Assimilation

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NCEP

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Many people have contributed to the GSI Hybrid/EnVar developments over the past several years. In particular, I would like to acknowledge Dave Parrish (GSI EnVar) and Jeff Whitaker (EnKF) for their significant contributions.

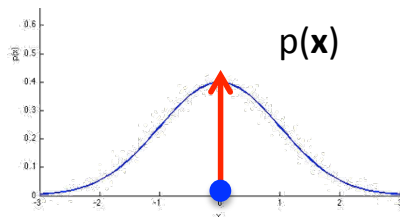
- Two main perspectives of practical data assimilation & hybrid approach

Variational Approach:

Least square estimation

[maximum likelihood]

- 3D-Var (3 dim in space)
- 4D-Var (4th dim is time)

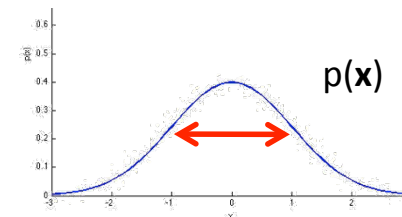


Sequential (KF) Approach:

Minimum Variance estimate

[least uncertainty]

- Optimal Interpolation (OI)
- (Extended / Ensemble)
Kalman Filter



HYBRID

Courtesy: Kayo Ide

Kalman Filter (Linear)

$$\begin{array}{l} \text{Forecast Step} \\ \text{Analysis} \end{array} \left\{ \begin{array}{l} \mathbf{x}_k^b = \mathbf{M}_k (\mathbf{x}_{k-1}^a) \\ \mathbf{B}_k = \mathbf{M}_k \mathbf{A}_{k-1} \mathbf{M}_k^T + \mathbf{Q}_k \\ \mathbf{x}_k^a = \mathbf{x}_k^b + \mathbf{K}_k (\mathbf{y}_k - \mathbf{H}_k \mathbf{x}_k^b) \\ \mathbf{K}_k = \mathbf{B}_k \mathbf{H}_k^T (\mathbf{R}_k + \mathbf{H}_k \mathbf{B}_k \mathbf{H}_k^T)^{-1} \\ \mathbf{A}_k = (\mathbf{I} - \mathbf{K}_k \mathbf{H}_k) \mathbf{B}_k \end{array} \right.$$

- Complete set of equations for DA cycling:
 - State **and** error covariances are propagated forward in time, and updated with observations at time k
 - Under assumptions of linearity (\mathbf{M} , \mathbf{H}), KF produces optimal set of analysis states
 - Analysis is the minimum variance estimate of the state

Kalman Filter for Large Dimensions

- Kalman filters (and EKF) are impractical for large system like NWP models
 - For present day NWP, the state size (N) can be $> O(10^8)$
- However, a variety of Kalman Filters have been developed for large dimensional systems
 - All of these rely on **Low-Rank** Approximations of the background and analysis error covariance matrices
- Assume that \mathbf{B}_k has rank $M \ll N$, so that we can write the error covariance as a function of \mathbf{X}^b ($N \times M$), where M can be ~ 100

$$\mathbf{B}_k = \mathbf{X}_k^b (\mathbf{X}_k^b)^T$$

Ensemble Approach to Represent $p(\mathbf{x})$

◆ Ensemble

Courtesy: Kayo Ide

- Members

$$\mathbf{X} = \{\mathbf{x}^{(m)}\} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(M)}\}$$

- Spread

$$\Delta\mathbf{X} = \{\mathbf{x}^{(m)} - \bar{\mathbf{x}}\} = \{\mathbf{x}^{(1)} - \bar{\mathbf{x}}, \dots, \mathbf{x}^{(M)} - \bar{\mathbf{x}}\}$$

- Mean

$$\bar{x}_n = \frac{1}{M} \sum_{m=1}^M x_n^{(m)}$$

$$\bar{\mathbf{x}} = \frac{1}{M} \sum_{m=1}^M \mathbf{x}^{(m)}$$

- Covariance

$$P_{nn} = \frac{1}{M-1} \sum_{m=1}^M (x_n^{(m)} - \bar{x}_n)^2$$

$$P_{in} = P_{ni} = \frac{1}{M-1} \sum_{m=1}^M (x_i^{(m)} - \bar{x}_i)(x_n^{(m)} - \bar{x}_n)$$

$$\mathbf{P} = \frac{1}{M-1} (\Delta\mathbf{X})(\Delta\mathbf{X})^T$$

◆ Issues

- Sampling of by ensemble can be poor, especially for

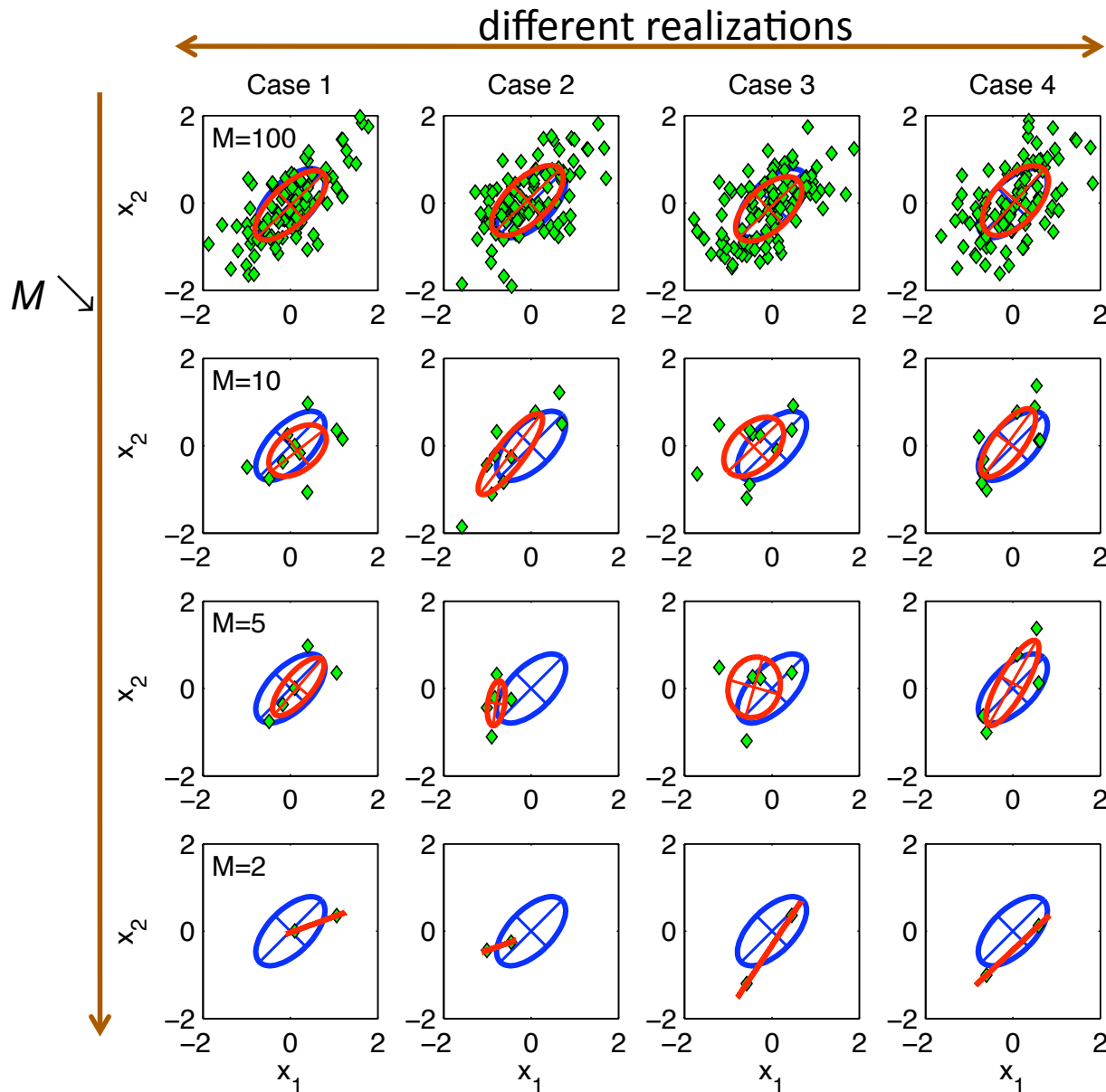
- Small M

- Small P_{in}

- Rank of \mathbf{P} is at most $M-1$

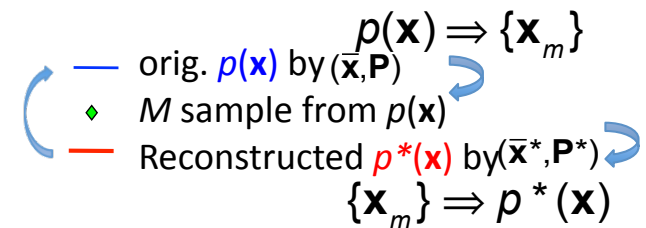
- There infinitely many $\Delta\mathbf{X}$ that have the same $\mathbf{P} = (1/M-1)\Delta\mathbf{X}(\Delta\mathbf{X})^T$

$p(\mathbf{x})$ Sampling & Reconstruction by Ensemble: 2D



Assuming Gaussian pdfs

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{N/2} |\mathbf{P}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \bar{\mathbf{x}})^T \mathbf{P}^{-1}(\mathbf{x} - \bar{\mathbf{x}})\right)$$



- If sampling is well-done, then $p^*(\mathbf{x}) \sim p(\mathbf{x})$.
- 'Fitness' of $p^*(\mathbf{x})$ to $p(\mathbf{x})$ vary case by case particularly for small M .
- All cases, $N \leq M$.

Courtesy: Kayo Ide

Ensemble Kalman Filters

More on these later today....

- Ensemble Kalman Filters (EnKF) are Monte Carlo approximations/implementations, using sample covariances from an ensemble (over bar represents ensemble mean):

$$\bar{\mathbf{x}}_k^b = \frac{1}{M} \sum_{m=1}^M (\mathbf{x}_{k,m}^b) \quad \mathbf{B}_k \approx \mathbf{B}_k^e = \mathbf{X}_k^b (\mathbf{X}_k^b)^T = \frac{1}{M-1} \sum_{m=1}^M (\mathbf{x}_{k,m}^b - \bar{\mathbf{x}}_k^b)(\mathbf{x}_{k,m}^b - \bar{\mathbf{x}}_k^b)^T$$

- Where \mathbf{X}_k^b is a matrix ($N \times M$) of ensemble forecast perturbations:

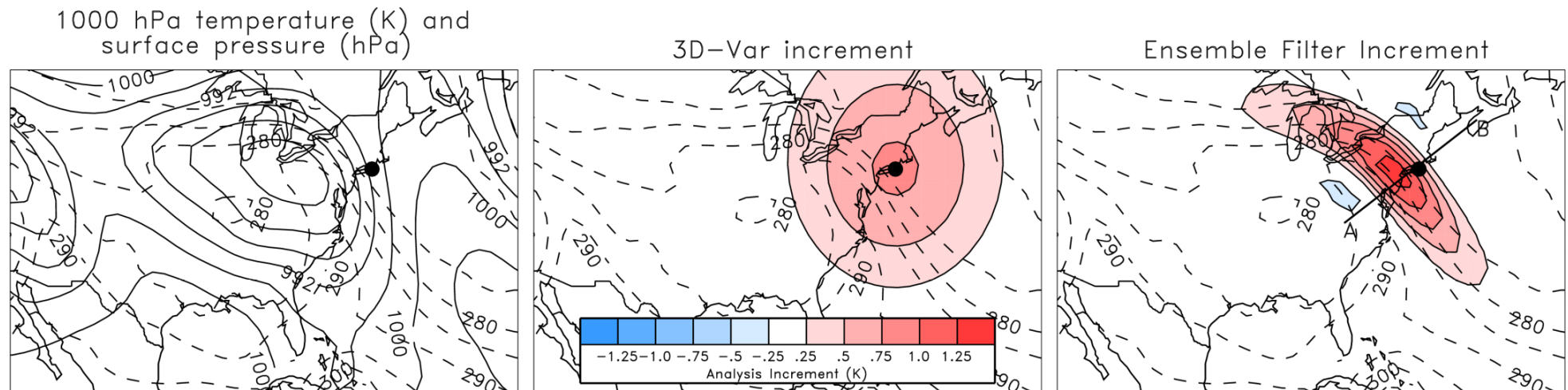
$$\mathbf{X}_k^b = \frac{1}{\sqrt{M-1}} \left((\mathbf{x}_{k,1}^b - \bar{\mathbf{x}}_k^b), (\mathbf{x}_{k,2}^b - \bar{\mathbf{x}}_k^b), \dots, (\mathbf{x}_{k,M}^b - \bar{\mathbf{x}}_k^b) \right)$$

- And the full \mathbf{B}^e is never explicitly computed! Instead, we represent it in the subspace of the $M \times M$ ensemble space.

What does B_e gain us?

Flow Dependence / Errors of the Day

Temperature observation near warm front



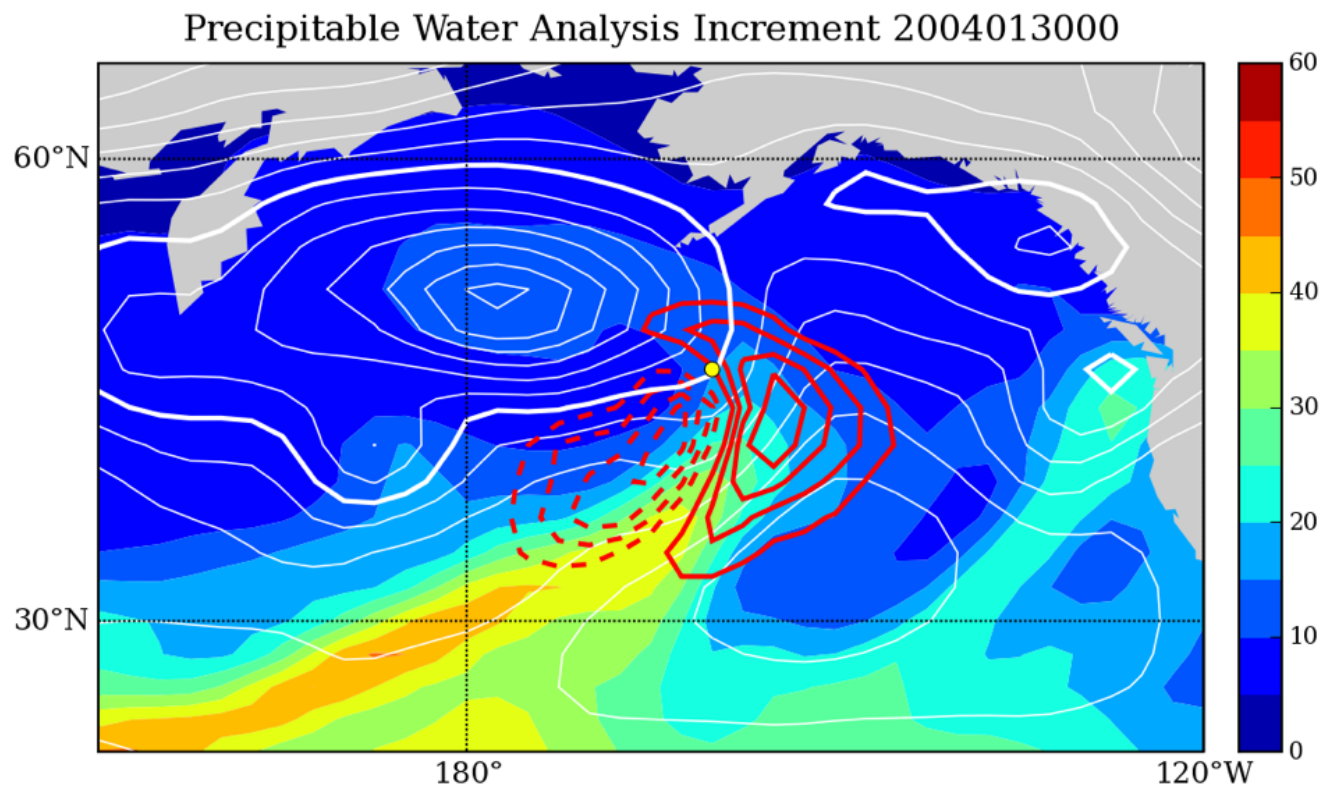
B_f

B_e

Courtesy: Jeff Whitaker

What does B_e gain us? Multivariate Correlations

Surface pressure observation near “atmospheric river”



First guess surface pressure (white contours) and precipitable water increment (A-G, red contours) after assimilating a single surface pressure observation (yellow dot) using B_e .

Courtesy: Jeff Whitaker

Use of \mathbf{B}^e in Var (GSI)

- If we had it, we could substitute ensemble estimate of error covariance

$$J_{\text{EnKF}}(\mathbf{x}'_k) = \frac{1}{2}(\mathbf{x}'_k)^T (\mathbf{B}^e)^{-1} (\mathbf{x}'_k) + \frac{1}{2}(\mathbf{y}'_o - \mathbf{H}\mathbf{x}'_k)^T \mathbf{R}^{-1} (\mathbf{y}'_o - \mathbf{H}\mathbf{x}'_k)$$

- This is in the full physical space, which we can work around by introducing a new control variable:

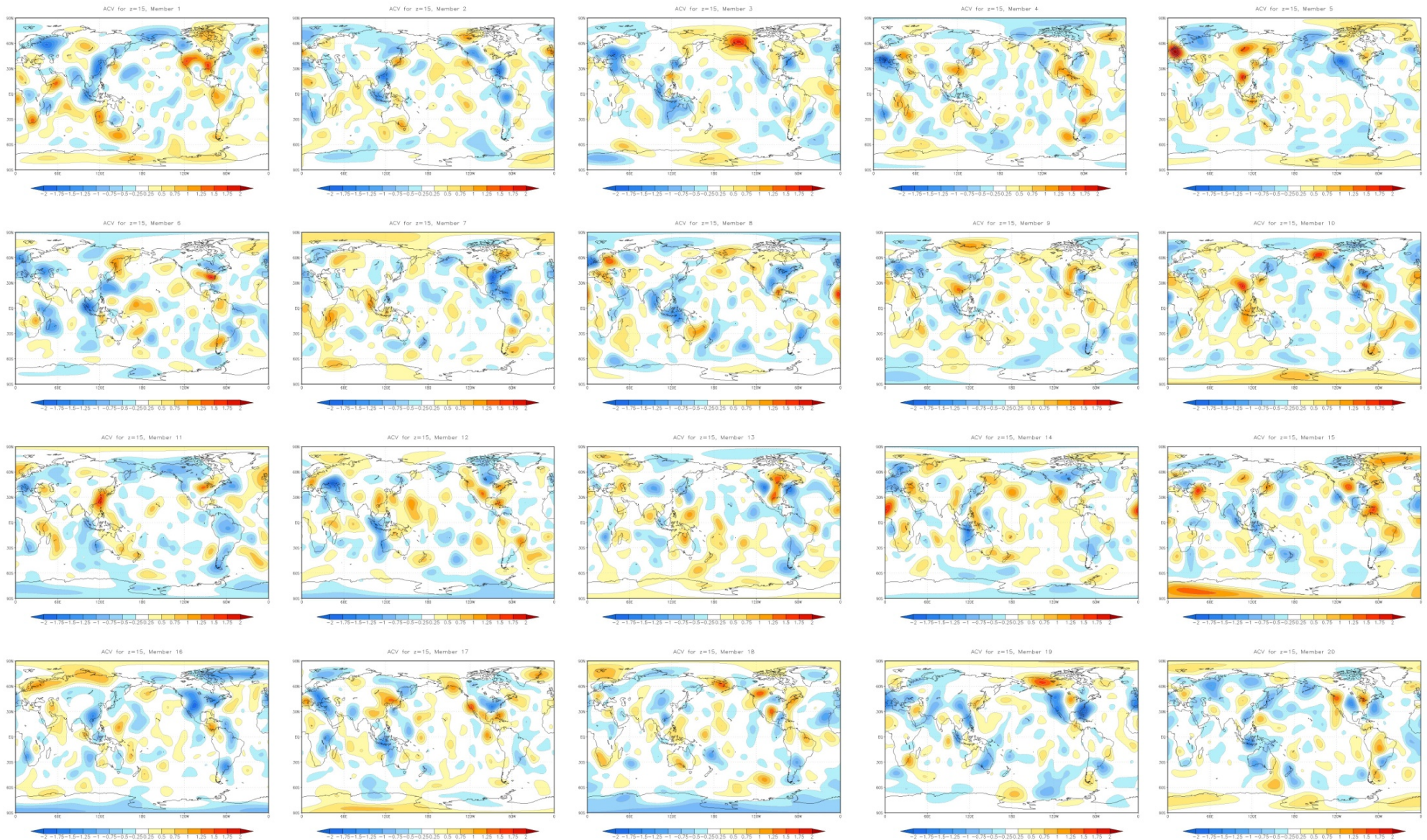
$$J_{\text{EnKF}}(\mathbf{x}'_k) = \frac{1}{2}(\alpha)^T \mathbf{L}^{-1} (\alpha) + \frac{1}{2}(\mathbf{y}'_o - \mathbf{H}\mathbf{x}'_k)^T \mathbf{R}^{-1} (\mathbf{y}'_o - \mathbf{H}\mathbf{x}'_k)$$

$$\mathbf{x}'_k = \sum_{m=1}^M (\alpha^m \circ \mathbf{x}_e^m)$$

- Where α is the local weight for the ensemble members
- \mathbf{L} is the **localization** on the extended control variable
- \mathbf{x}_e are the ensemble perturbations that represent \mathbf{B}^e (as in EnKF)



Control Variable Example (2012012212, z=15, 20 members)



- Linearly combine full rank (static) and flow-dependent (ensemble) background error covariance estimates

$$\mathbf{B}^h = (1 - \beta) \mathbf{B}^e + \beta \mathbf{B}^c$$

- Solution in Var: Add a second background term (one for ensemble, and one for static). Here, we'll denote the climatological (c) and ensemble (e) contributions

$$J_{\text{Hyb}}(\mathbf{x}_c, \alpha) = \beta_c \frac{1}{2} (\mathbf{x}'_c)^T \mathbf{B}^c (\mathbf{x}'_c) + \beta_e \frac{1}{2} (\alpha)^T \mathbf{L}^{-1} (\alpha) + \frac{1}{2} (\mathbf{y}'_o - \mathbf{H} \mathbf{x}'_t)^T \mathbf{R}^{-1} (\mathbf{y}'_o - \mathbf{H} \mathbf{x}'_t)$$

$$\mathbf{x}'_t = \mathbf{x}'_f + \sum_{m=1}^M (\alpha^m \circ \mathbf{x}_e^m)$$

$$J_{\text{Hyb}}(\mathbf{x}_c, \alpha) = \underbrace{\beta_c \frac{1}{2} (\mathbf{x}'_c)^T \mathbf{B}^c (\mathbf{x}'_c)}_{\text{clim. (var)}} + \underbrace{\beta_e \frac{1}{2} (\alpha)^T \mathbf{L}^{-1} (\alpha)}_{\text{ensemble covariance}} + \underbrace{\frac{1}{2} (\mathbf{y}'_o - \mathbf{H} \mathbf{x}'_t)^T \mathbf{R}^{-1} (\mathbf{y}'_o - \mathbf{H} \mathbf{x}'_t)}_{\text{data fit}}$$

$$\mathbf{x}'_t = \mathbf{x}'_f + \sum_{m=1}^M (\alpha^m \mathbf{x}_e^m)$$

β_c & β_e : weighting coefficients for clim. (var) and ensemble covariance respectively

\mathbf{x}'_t : (total increment) sum of increment from fixed/static $\mathbf{B}(\mathbf{x}'_c)$ and ensemble \mathbf{B}

α_k : extended control variable; \mathbf{x}_e^m : ensemble perturbations

- analogous to the weights in the LETKF formulation

$$(\mathbf{w}_{k,m} = (\mathbf{Y}_{k,m}^b)^T [\mathbf{Y}_{k,m}^b (\mathbf{Y}_{k,m}^b)^T + \mathbf{R}]^{-1} \mathbf{d}_k)$$

\mathbf{L} : correlation matrix [effectively the localization of ensemble perturbations]

With Preconditioning

$$\mathbf{v}^m = \beta_e \mathbf{L}^{-1} \alpha^m \quad \mathbf{z} = \beta_c \mathbf{B}_c^{-1} \mathbf{x}'_c$$

$$J(\mathbf{z}, \mathbf{v}) = \frac{1}{2} (\mathbf{x}'_c)^\top \mathbf{z} + \frac{1}{2} \alpha^\top \mathbf{v} + J_o$$

$$\mathbf{x}'_c = (\beta_c)^{-1} \mathbf{B}_c \mathbf{z} \quad \alpha = (\beta_e)^{-1} \mathbf{L} \mathbf{v}$$

For the double Conjugate Gradient (GSI default), inverses of \mathbf{B} and \mathbf{L} not need and the solution is preconditioned by full \mathbf{B} .

This formulation differs from the UKMO and Canadians, who use a square root formulation. Also, the weights can be applied to the increments themselves:

$$\mathbf{x}'_t = \beta_c \mathbf{x}'_c + \beta_e \sum_{m=1}^M (\alpha^m \circ \mathbf{x}_e^m)$$

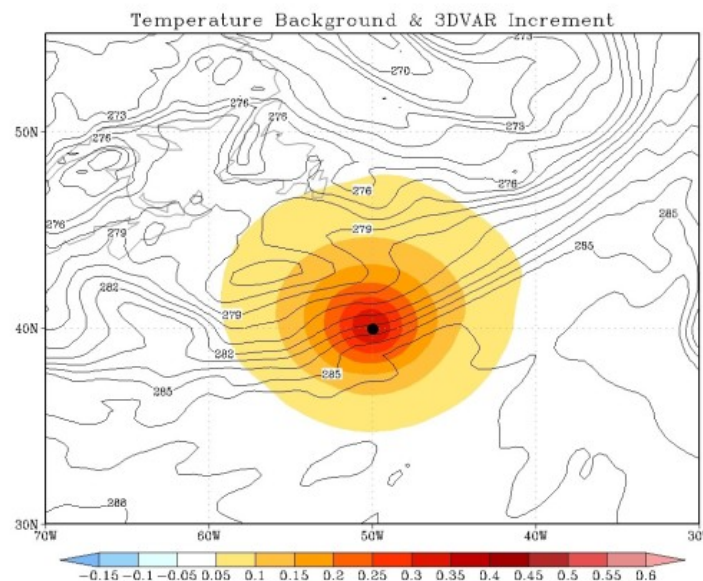
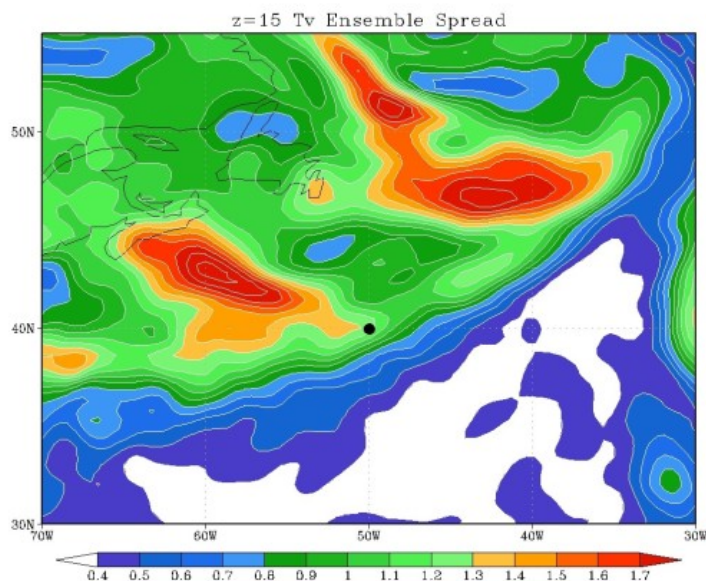
Hybrid: Variational methods that combine **static** and **ensemble** covariances.

EnVar: Variational methods using ensemble covariances

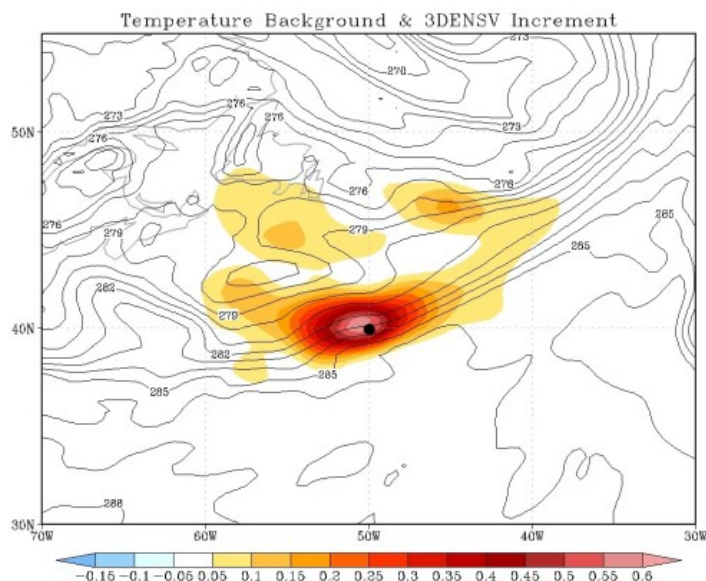
Hybrid 4DVar: Variational method using a combination of **static** and **ensemble** covariances at the beginning of the window, but using a **tangent-linear** and **adjoint** model

Hybrid 4DEnVar: Variational method using a combination of **static** and **ensemble** covariances at the all times in the window, *without* the need of a **tangent-linear** or **adjoint**

Single Temperature Observation



3DVAR

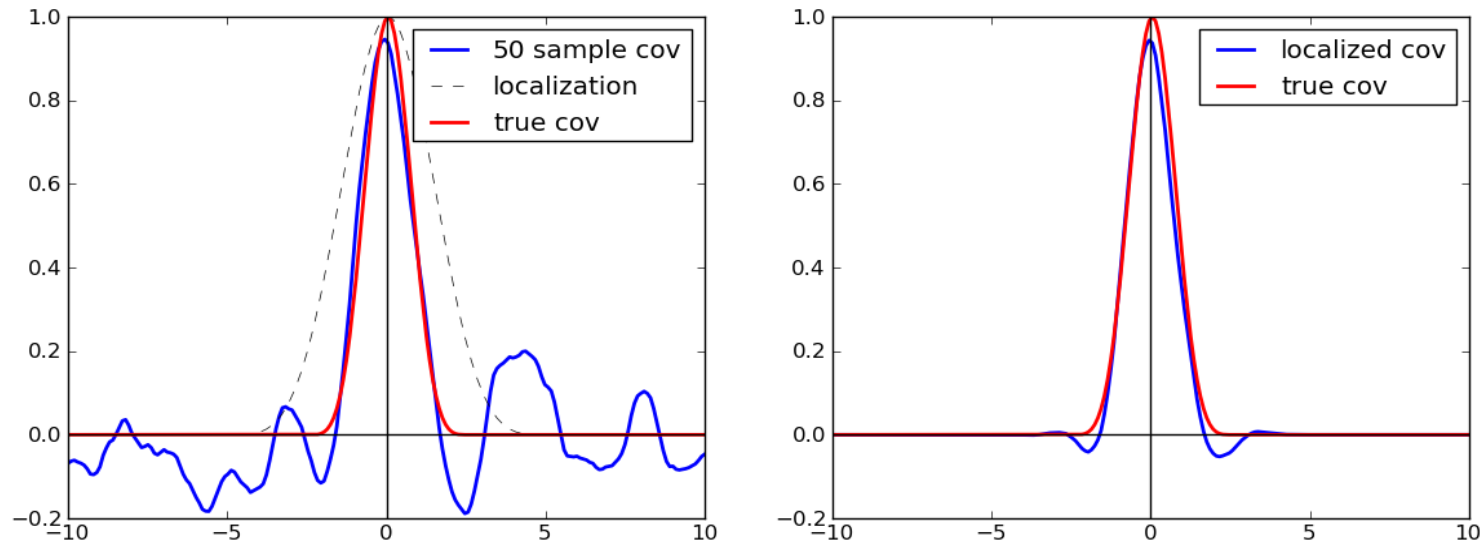


EnVar

So what's the catch?

- Most configurations of hybrid DA systems require the development and maintenance of two DA systems
 - EnKF + Var
- Still need to deal with *localization* and other sampling-related issues (though somewhat mitigated by use of full rank \mathbf{B}_c)
 - Rank deficiency: Using small ensemble size to represent something of much larger dimension
- Even more parameters to explore
 - Trade off between ensemble size, resolution, hybrid weights, etc.

Example of Covariance Localization



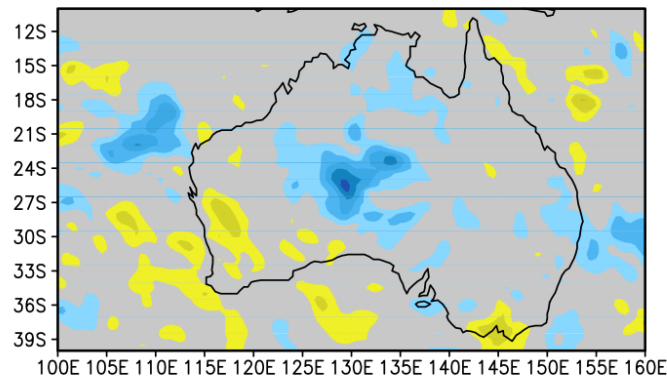
Estimates of covariances from a small ensemble will be noisy, with signal to noise small especially when covariance is small

Courtesy: Jeff Whitaker

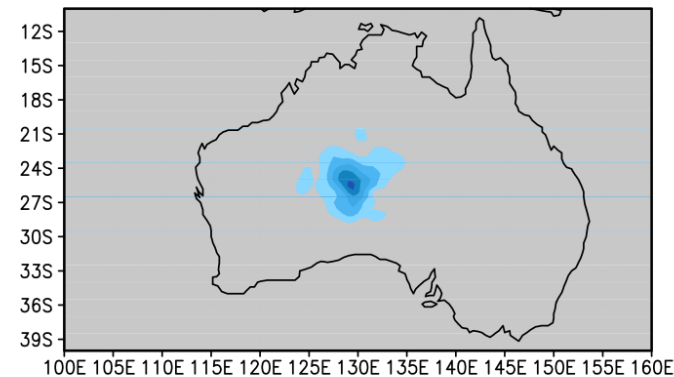
NWP Localization Example

Temperature Covariance with Temperature ob

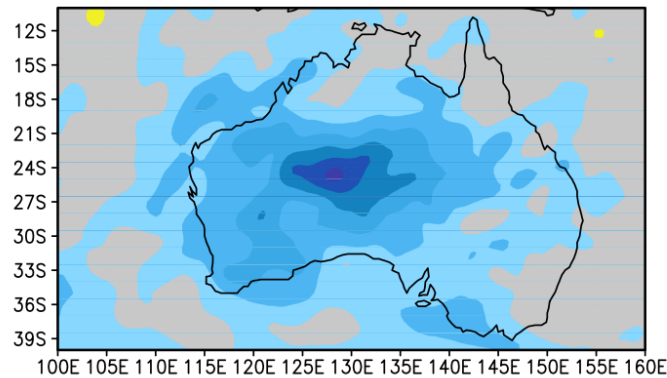
T 850



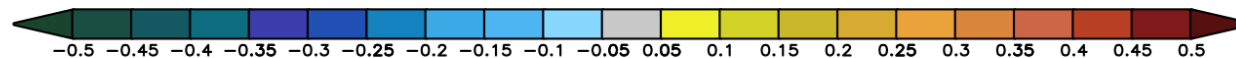
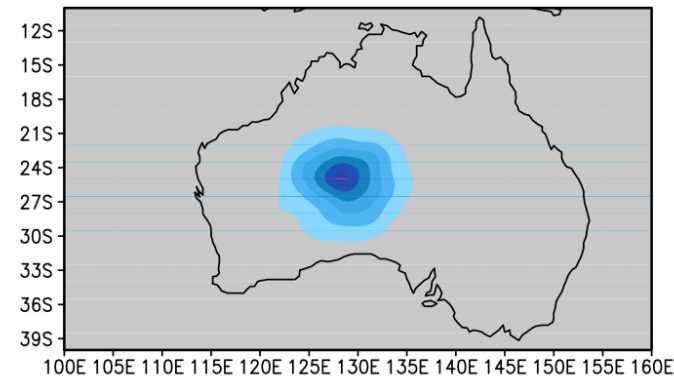
T 850 with Localization



T 10



T 10 with Localization



Courtesy: Jeff Whitaker

GSI Hybrid Configuration

- Hybrid related parameters controlled via GSI namelist **&hybrid_ensemble**
- Logical to turn on/off hybrid ensemble option (**l_hyb_ens**)
- Ensemble size (**n_ens**), resolution (**jcap_ens**, **nlat_ens**, **nlon_ens**)
- Source of ensemble: GFS spectral, native model, etc.
(**regional_ensemble_option**)
- Weighting factor for static contribution to increment (**beta_s0**)
 - Option to specify different beta weights as a function of vertical level
(**readin_beta**)
- Horizontal and vertical distances for localization, via **L** on augmented control variable (**s_ens_h**, **s_ens_v**)
 - Localization distances are the same for all variables since operating on α .
i.e. no variable localization
 - Option to specify different localization distances as a function of vertical level (**readin_localization**)
- Other regional options related to resolution, pseudo ensemble, etc.

Notes on some GSI Hybrid Options

- **beta_s0**
 - If weights set this way, code will assume that ensemble beta will be 1-beta_s0
 - If set via readin_beta, the ensemble + climatological beta weights do not have to sum to one for a given level (error tuning)
- **s_ens_h**
 - Horizontal decorrelation distance in km (Gaussian half-width, not zero-distance)
- **s_ens_v**
 - If > 0, vertical decorrelation given in units of model layers
 - If < 0, vertical decorrelation given in units of $d \ln p$ (scale height)
 - i.e. s_ens_v=-0.5 actually means 0.5 in units of $d \ln p$
- **filename**
 - If using global (GFS) ensemble, will generally follow sigfHH_ens_memNNN
 - HH = forecast hour
 - NNN = integer ensemble member number
- **Regional specific**
 - Regional_ensemble_option, grid_ratio_ens, more....

Example: global_hybens_info.l64.txt

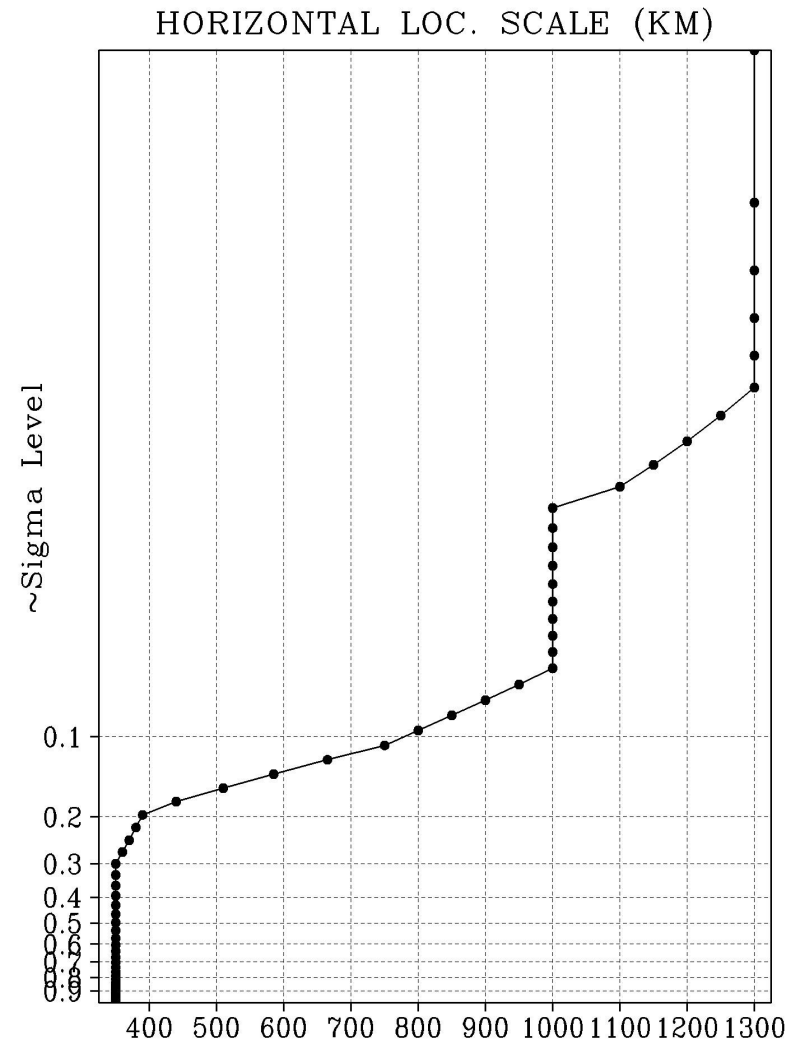
64				# of levels			
350.0	-0.5	0.1250	0.8750	s_ens_h(1)	s_ens_v(1)	beta_s0(1)	beta_e(1)
350.0	-0.5	0.1250	0.8750	s_ens_h(2)	s_ens_v(2)	beta_s0(2)	beta_e(2)
350.0	-0.5	0.1250	0.8750	s_ens_h(3)	s_ens_v(3)	beta_s0(3)	beta_e(3)
350.0	-0.5	0.1250	0.8750	s_ens_h(4)	s_ens_v(4)	beta_s0(4)	beta_e(4)
350.0	-0.5	0.1250	0.8750	s_ens_h(5)	s_ens_v(5)	beta_s0(5)	beta_e(5)
350.0	-0.5	0.1250	0.8750	s_ens_h(6)	s_ens_v(6)	beta_s0(6)	beta_e(6)
.				.			
.				.			
.				.			
1300.0	-0.5	0.1250	0.8750	s_ens_h(63)	s_ens_v(63)	beta_s0(63)	beta_e(63)
1300.0	-0.5	0.1250	0.8750	s_ens_h(64)	s_ens_v(64)	beta_s0(64)	beta_e(64)

- **Localization:**
 - Horizontal: Spectral operator to apply Gaussian function. Localization distances function of model vertical level
 - Option for RF-based horizontal localization (for regional applications)
 - Vertical: Recursive filter (separable from above)
- **Ensemble variables:** Can be different than standard control variable for **Bc** (Default $u, v, T, ps, q_{wv}, q_{oz}, q_{cw}$)
 - `ensctl2state` and `state2ensctl` does mapping between state space and ensemble variables
- **Dual Resolution:** If ensemble at lower resolution, interpolation (and adjoint) between ensemble/analysis grids* [**T**]
- **Initialization:** Option for Tangent Linear Normal Mode Constraint [**C**]

$$\mathbf{x}'_t = \mathbf{C} \left[\mathbf{x}'_f + \mathbf{T} \sum_{m=1}^M (\alpha^m \circ \mathbf{x}_e^m) \right]$$

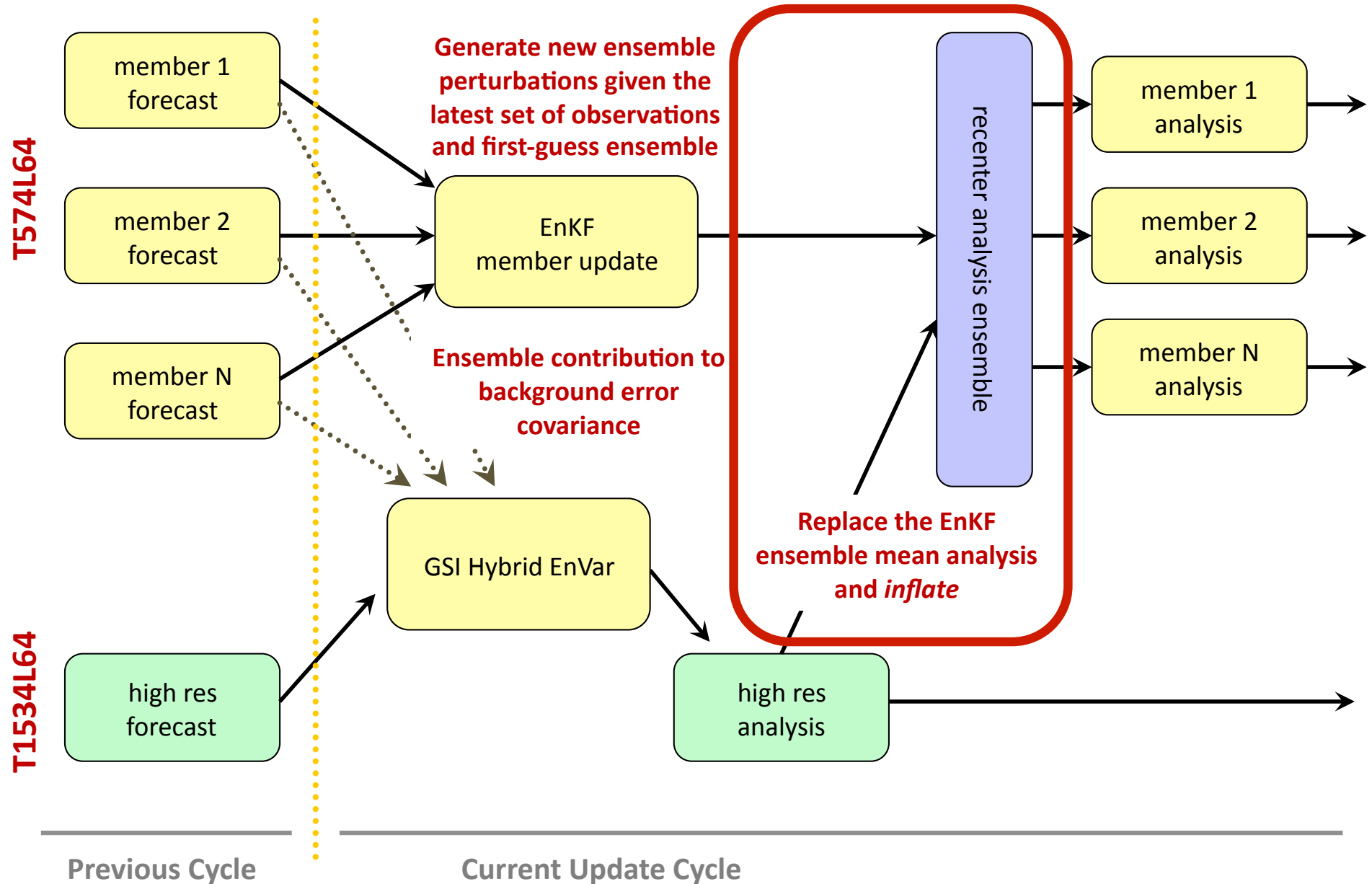
Current Hybrid for GDAS/GFS

- T1534L64 Deterministic (SL dynamics)
 - T574L64 EnSRF, 80 members, Stoch. Physics, Hourly Output
- 87.5% ensemble, 12.5% climatological for hybrid increment
- Level dependent horizontal localization (divide by 0.38 to convert to GC zero distance)
 - 0.5 scale heights in vertical





Dual-Res Coupled Hybrid Var/EnKF Cycling



What if I am not running an EnKF?

- In principle any ensemble can be used;
 - so long as the ensemble represents the forecast errors well.
- GSI can ingest GFS global ensemble to update regional models
 - WRFARW/NMM, NAM, RR, HWRF
- 80 member GFS/EnKF 6h ensemble forecasts are archived at NCEP since May 2012.
 - Real time ensemble is also publicly available.

Ensemble of Data Assimilations

- Much like the stochastic EnKF, ECMWF and Meteo-France use an ensemble of data assimilations instead of an EnKF
 - Perturb the observations and model
 - Designed to represent and estimate the uncertainty in their deterministic 4DVAR
- This provides flow-dependent estimates of analysis error for their EPS
- Also provides flow-dependent estimates of background error for use in DA (either as \mathbf{B}_0 or in hybrid)
- Can be hugely expensive, given that a variational (4DVAR) update has to be executed for each ensemble member!



4D Hybrids

The Hybrid EnVar cost function can be easily extended to 4D and include a static contribution (ignore preconditioning)

$$J(\mathbf{x}'_c, \alpha) = \beta_c \frac{1}{2} (\mathbf{x}')^T \mathbf{B}_c^{-1} (\mathbf{x}') + \beta_e \frac{1}{2} \alpha^T \mathbf{L}^{-1} \alpha + \underbrace{\frac{1}{2} \sum_{k=1}^K (\mathbf{y}'_k - \mathbf{H}_k \mathbf{x}'_k)^T \mathbf{R}_k^{-1} (\mathbf{y}'_k - \mathbf{H}_k \mathbf{x}'_k)}_{\text{Jo term divided into observation "bins" as in 4DVAR}}$$

Jo term divided into observation
“bins” as in 4DVAR

Where the 4D increment is prescribed through linear combinations of the 4D ensemble perturbations plus static contribution, i.e. it is not itself a model trajectory

$$\mathbf{x}'_k = \mathbf{C}_k [\mathbf{x}'_c + \sum_{m=1}^M (\alpha^m \circ (\mathbf{x}'_e)_k^m)]$$

Here, static contribution is time invariant. \mathbf{C} represents TLNMC balance operator. No TL/AD in Jo term (\mathbf{M} and \mathbf{M}^T)

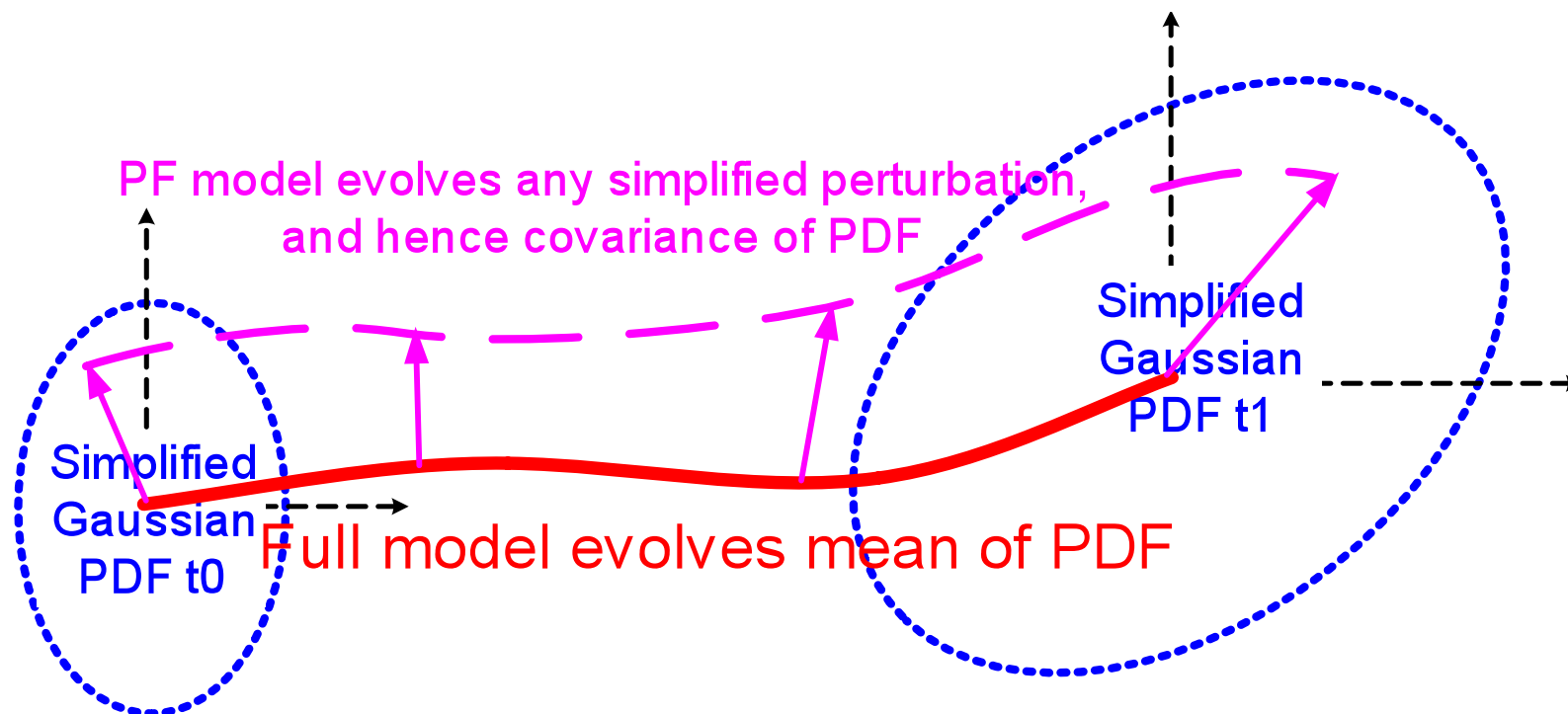
The traditional 4DVar cost function can be manipulated to use an ensemble to help prescribe the error covariance at the beginning of the window

$$J(\mathbf{x}'_c, \alpha) = \beta_c \frac{1}{2} (\mathbf{x}')^T \mathbf{B}_c^{-1} (\mathbf{x}') + \beta_e \frac{1}{2} \alpha^T \mathbf{L}^{-1} \alpha + \frac{1}{2} \sum_{k=1}^K (\mathbf{y}'_k - \mathbf{H}_k \mathbf{M}_k \mathbf{x}'_0)^T \mathbf{R}_k^{-1} (\mathbf{y}'_k - \mathbf{H}_k \mathbf{M}_k \mathbf{x}'_0)$$

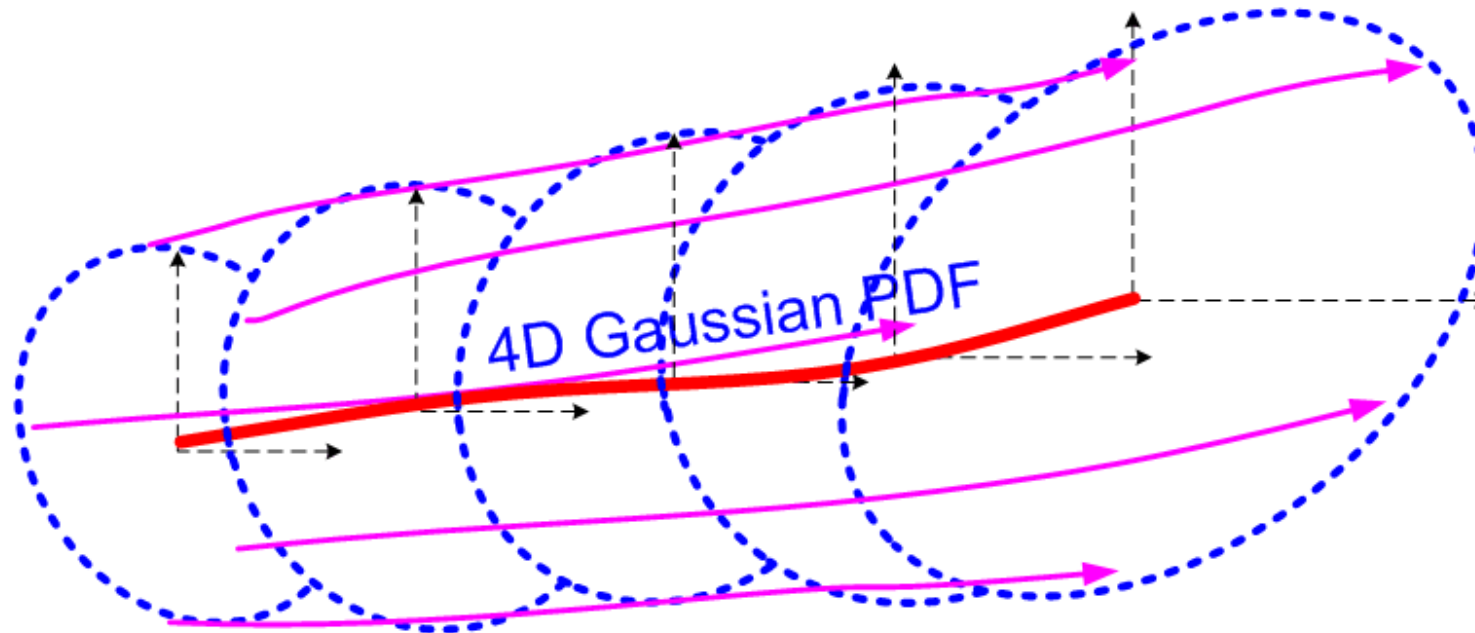
Jo term divided into observation
“bins” as in 4DVAR

$$\mathbf{x}'_0 = [\mathbf{x}'_c + \sum_{m=1}^M (\alpha^m \circ (\mathbf{x}_e)^m)]$$

Here, the hybrid error covariance is applied at the beginning of the window, and the TL/AD propagate within observation window (\mathbf{M} and \mathbf{M}^T) in Jo term



Lorenc & Payne 2007



Trajectories of perturbations from ensemble mean

Full model evolves mean of PDF

Localised trajectories define 4D PDF of possible increments

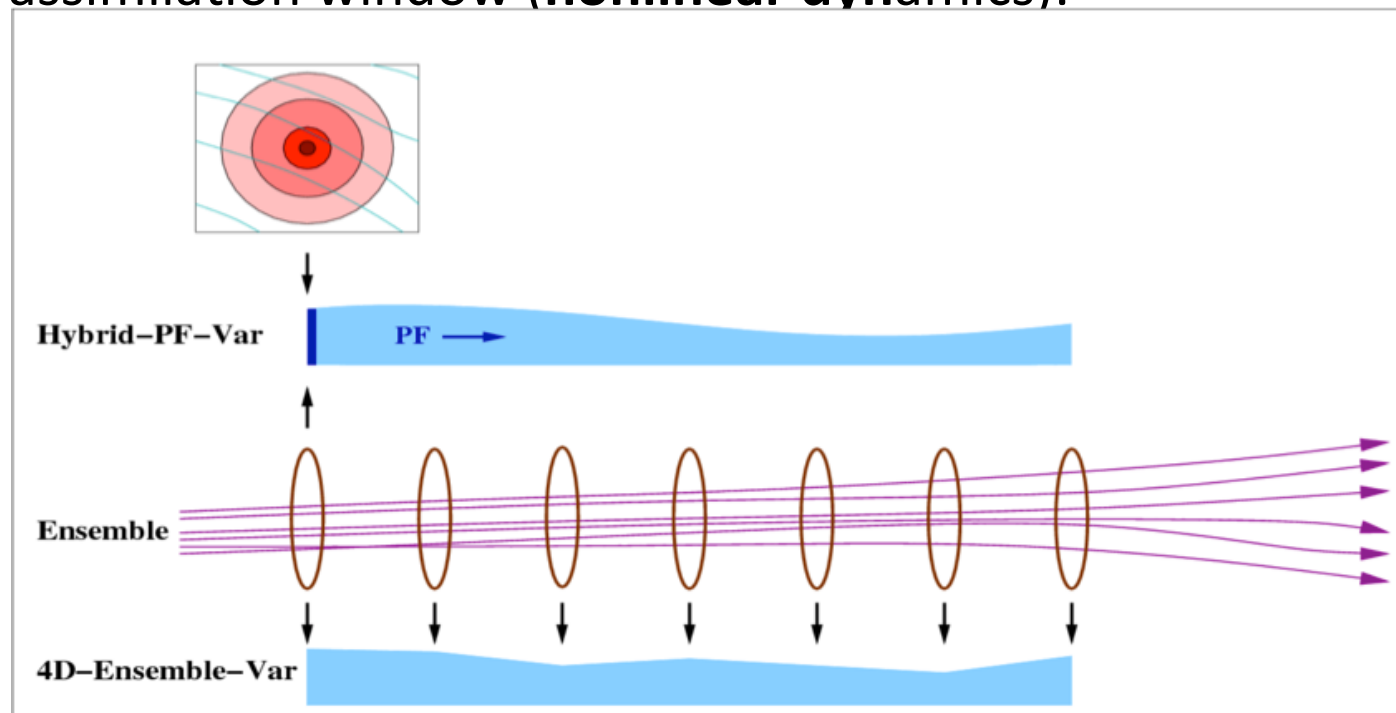
4D analysis is a (localised) linear combination of nonlinear trajectories. It is not itself a trajectory.

Courtesy: Andrew Lorenc

4D Hybrids

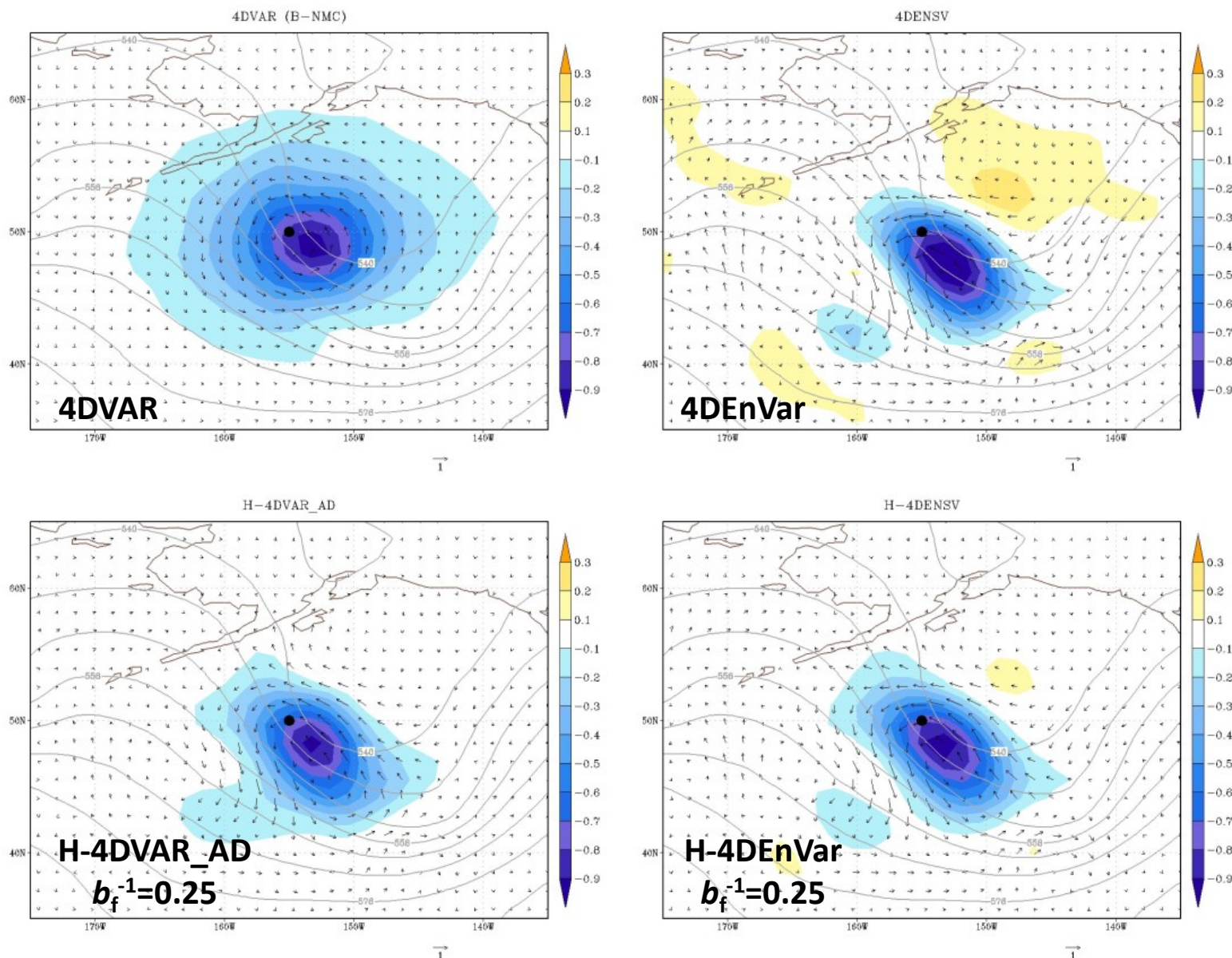
In the alpha control variable method one uses the ensemble perturbations to estimate \mathbf{P}^b only at the start of the 4DVar assimilation window: the evolution of \mathbf{P}^b inside the window is due to the **tangent linear dynamics** ($\mathbf{P}^b(t) \approx \mathbf{M}\mathbf{P}^b\mathbf{M}^T$)

In **4D-EnVar** \mathbf{P}^b is sampled from ensemble trajectories throughout the assimilation window (**nonlinear dynamics**):

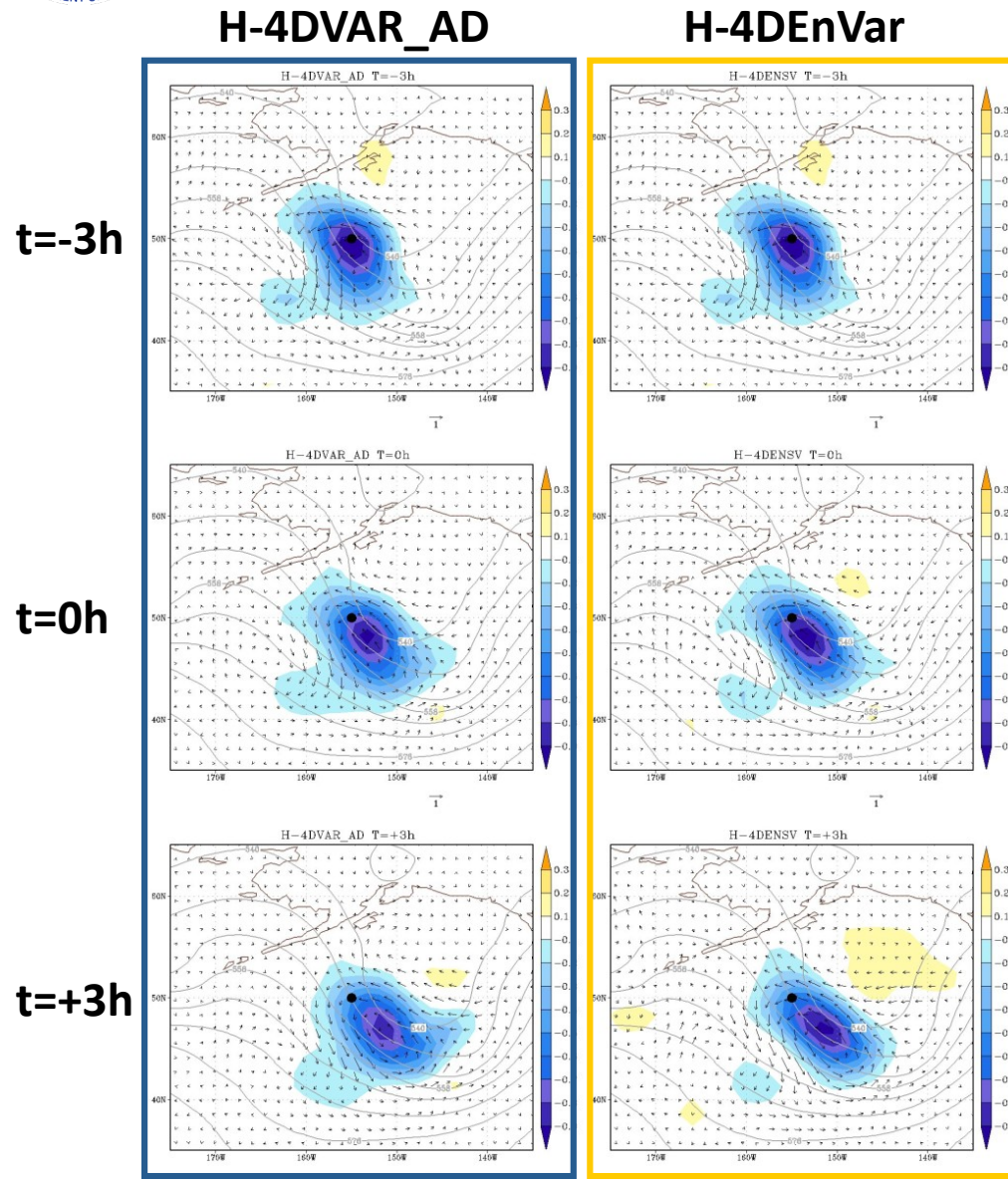


from: D. Barker &
A. Clayton
(UKMO)

Single Observation (-3h) Example for 4D Variants



Time Evolution of Increment



Solution at beginning of window same to within round-off (because observation is taken at that time, and same weighting parameters used)

Evolution of increment qualitatively similar between dynamic and ensemble specification

- **l4densvar**
 - Logical switch to turn on 4DVar
- **ens_nstarthr**
 - First forecast hour for ensemble valid in assimilation window. For the GDAS 06 hour cadence and window, this is “03”, i.e. to use sigf03-sigf09 ensemble
- **nh_r_obsbin**
 - Integer width for observation windows. GDAS uses hourly (“01”).
- **lwrite4danl**
 - Option to write out 4D analysis (guess+increment at interval of nh_r_obsbin).
- **thin4d**
 - Modify observation thinning to be a function of space only (no preferential treatment of observations near center of window)
- **filename**
 - Same as previously noted, but with multiple time levels consistent with above
- **l4dvar**
 - *Logical switch to turn on 4DVar (using TL/AD). User needs to compile with TL/AD interfaced to solver.*
 - *Can run hybrid En-4DVar using this option plus hybrid options (*not* l4densvar).*

- 4DVar is more comparable in cost to 3DVar/3DVar since it does not involve TL/AD
 - 4DVar can be at least 10x more expensive depending on configuration
 - Lots of cost in ensemble, much more IO (4D), etc.
- Standard practice to use middle-loop option (relinearization), but work to be done in exploring use of outer loop as in 4DVar
- Lots of work to do on multi-scale and scale-dependence
 - Localization
 - Hybrid weighting

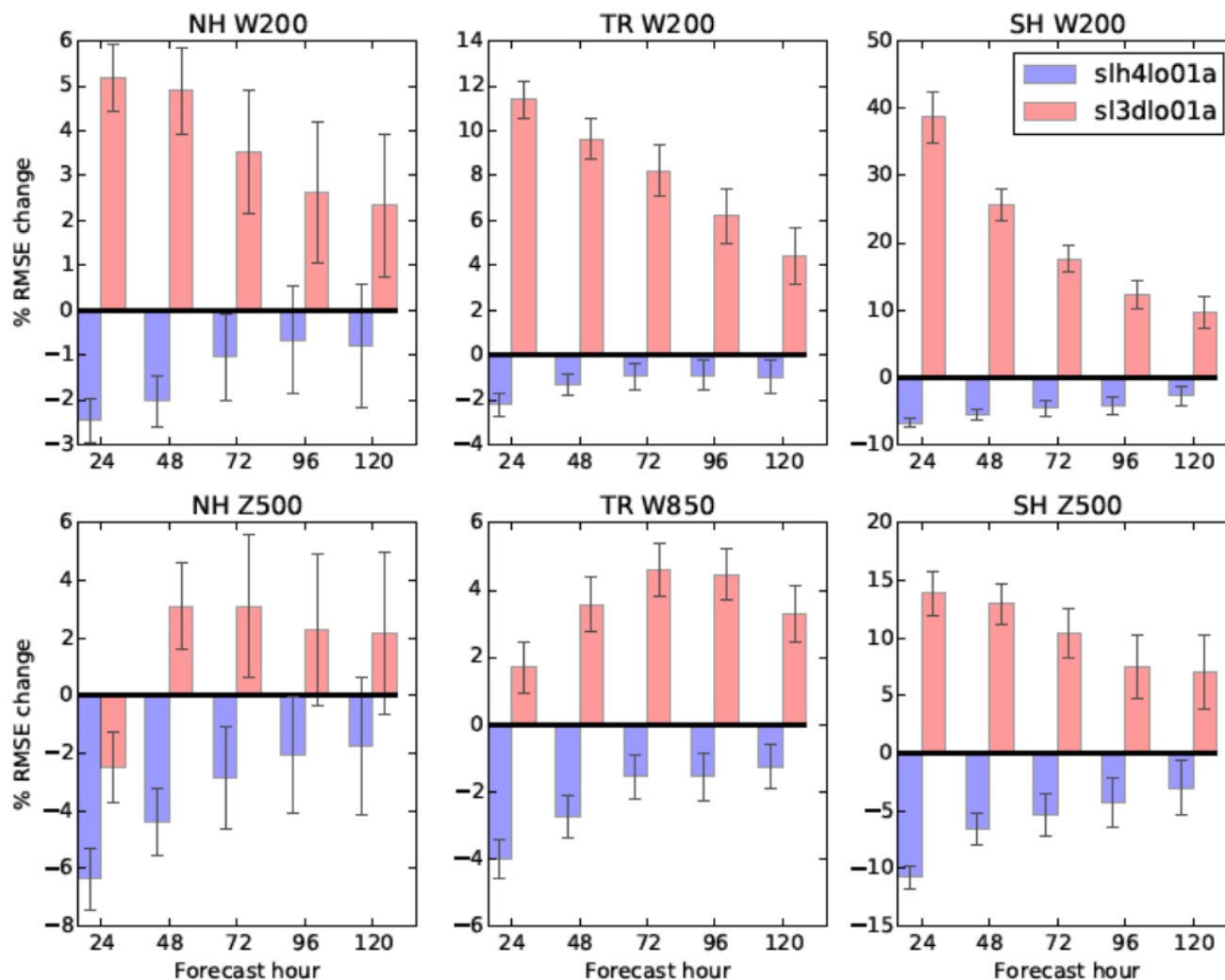


Global 4D Hybrid at Major NWP Centers



- Hybrid 4D EnVar
 - CMC (Canada)
 - Replaced 4DVAR
 - NCEP
 - Extension of hybrid 3DEnVar
- Hybrid En-4DVAR (Operational or in Testing)
 - UKMO
 - ECMWF*
 - Meteo-France*
 - US Navgem
 - JMA

3DVar / H3DEnVar / H4DEnVar



- Move from 3D Hybrid (current operations) to Hybrid 4D-EnVar yields improvement that is about 75% in amplitude in comparison from going to 3D Hybrid from 3DVAR.

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Questions?