EnKF overview

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3DVar Cost function

$$J(\delta \mathbf{x}) = \frac{1}{2}\delta \mathbf{x}^{\mathbf{T}}\mathbf{B}^{-1}\delta \mathbf{x} + \frac{1}{2}(\mathbf{H}\delta \mathbf{x} - \mathbf{d})^{\mathbf{T}}\mathbf{R}^{-1}(\mathbf{H}\delta \mathbf{x} - \mathbf{d})$$

J : Penalty (Fit to background + Fit to observations)

δx : Analysis increment ($\mathbf{x}^a$ – $\mathbf{x}^b$)

$\mathbf{x}^a$, $\mathbf{x}^b$: Analysis, Background

B : Background error covariance (estimated offline)

H : Observations (forward) operator

R : Observation error covariance (Instrument + representativeness)

$\mathbf{d} = \mathbf{y}^o - \mathbf{H}\mathbf{x}^b$, where $\mathbf{y}^o$ are the observations

Cost function (*J*) is minimized to find solution, **δx** [$\mathbf{x}^a = \mathbf{x}^b + \delta\mathbf{x}$]

Hybrid Ensemble Var Cost function

$$J_{\mathbf{hybrid}}\left(\delta\mathbf{x}\right)=\frac{\beta}{2}\boldsymbol{\delta}\mathbf{x}^{\mathrm{T}}\mathbf{B}_{s}^{-1}\boldsymbol{\delta}\mathbf{x}+\frac{1-\beta}{2}\boldsymbol{\delta}\mathbf{x}^{\mathrm{T}}\mathbf{B}_{e}^{-1}\boldsymbol{\delta}\mathbf{x}+\frac{1}{2}\left(\mathbf{H}\boldsymbol{\delta}\mathbf{x}-\mathbf{d}\right)^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{H}\boldsymbol{\delta}\mathbf{x}-\mathbf{d}\right)$$

$\mathbf{B}_s$: (**Static**) background-error covariance (estimated offline)

$\mathbf{B}_e$: (**Flow-dependent**) background-error covariance (estimated from ensemble)

β: Weighting factor (0.25 means total **B** is ¾ ensemble).

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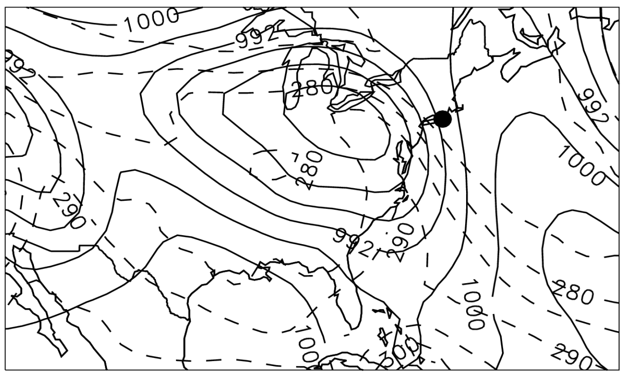
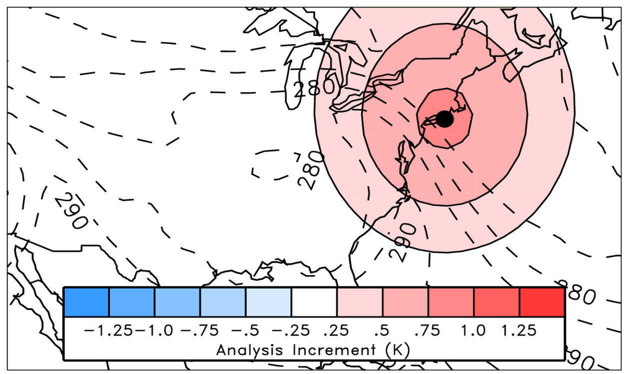
What does $\mathbf{B_e}$ do?

Temperature observation near a warm front

1000 hPa temperature (K) and surface pressure (hPa)

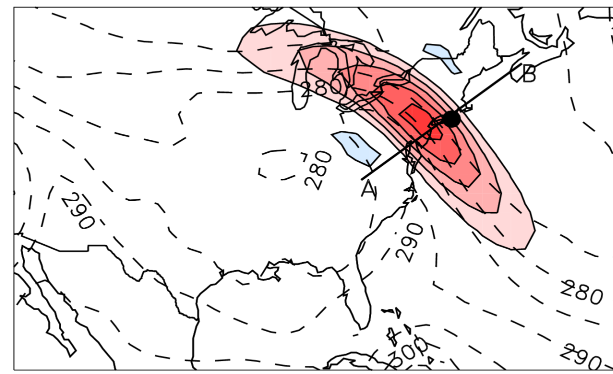


Increment (all static)



$\mathbf{B_s}$

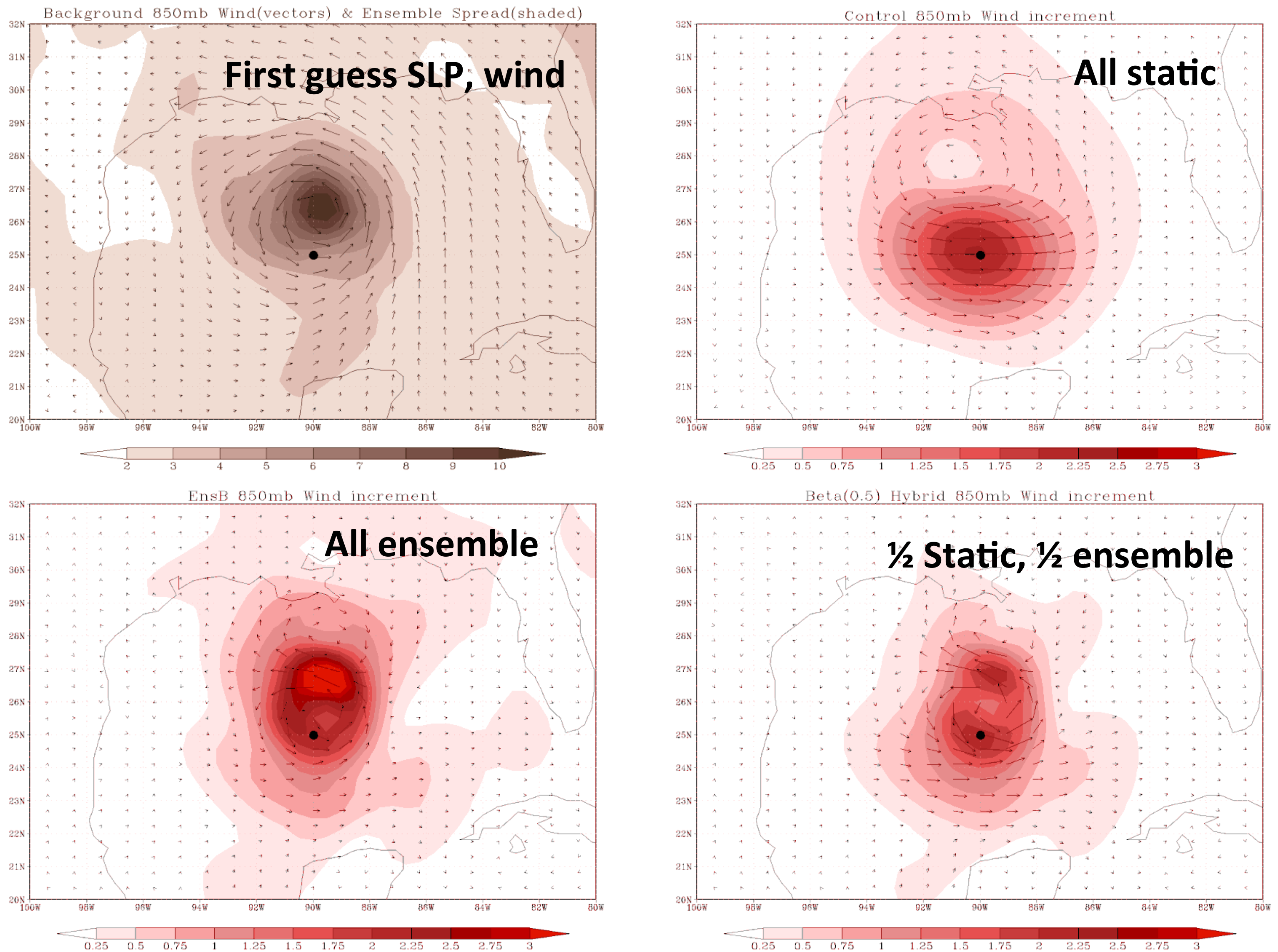
Increment (all ensemble)



$\mathbf{B_e}$

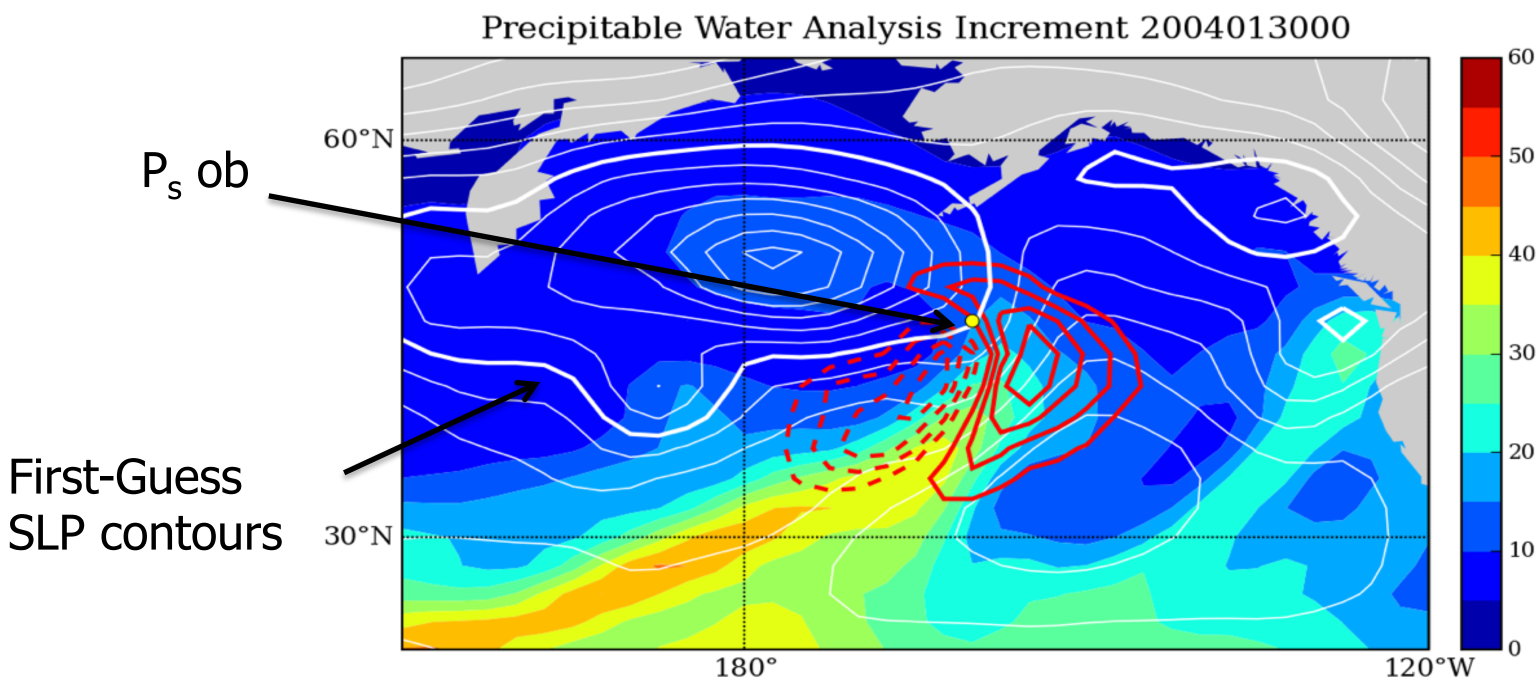
What does $\mathbf{B}_e$ do?

Zonal wind observation near a hurricane (Ike)



What does $\mathbf{B}_e$ do?

Surface pressure observation near an “atmospheric river”



3DVar increment would be zero!

(*cross-variable covariances hard to model with static* $\mathbf{B}_s$)

What does $\mathbf{B}_e$ do?

- Adds **situation-dependence** to analysis increments.
- Sparse observations near coherent dynamical features used more effectively.
- Changes in the observing network can be captured in background-error variance.
- ***More information extracted from observations => More skillful forecasts***

So what’s the catch?

- Rank Deficiency
  - Need a **fairly large O(100)** ensemble to represent uncertainty
    - Too few degrees of freedom available to fit the observations
    - Low rank approximation yields spurious long-distance correlations

- Mistreatment of “system error/uncertainty”
  - **Sampling (as above), model error, observation operator error, representativeness, etc.**

- State estimate is ensemble average
  - This can produce **unphysical estimates**, smooth out high fidelity information, etc.

So what's the catch?

- The GSI variational system does not provide the ensemble – it provides an analysis that can be interpreted as the ensemble mean, given an ensemble that represents forecast uncertainty.
- In NCEP operations, an "Ensemble Kalman Filter" (EnKF) is used to generate the background ensemble.

Data assimilation terminology

- **y** : Observation vector (weather balloons, satellite radiances, etc.)
- **x** : the state of the atmosphere as represented by the model
- $\mathbf{x}^b$: Background state vector ("prior")
- $\mathbf{x}^a$: Analysis state vector ("posterior")
- **H** : (hopefully linear) operator to convert model state → observation location & type
- **R** : Observation - error covariance matrix
- **$\mathbf{P}^b$: Background - error covariance matrix**
- $\mathbf{P}^a$: Analysis - error covariance matrix

Approaches to Solution

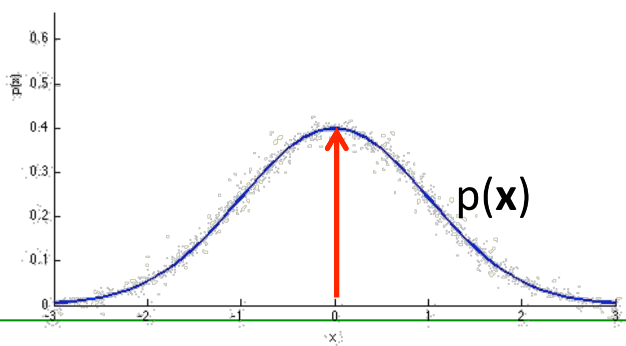
- Two main perspectives of practical data assimilation & hybrid approach

Variational Approach:

Least square estimation

[maximum likelihood]

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

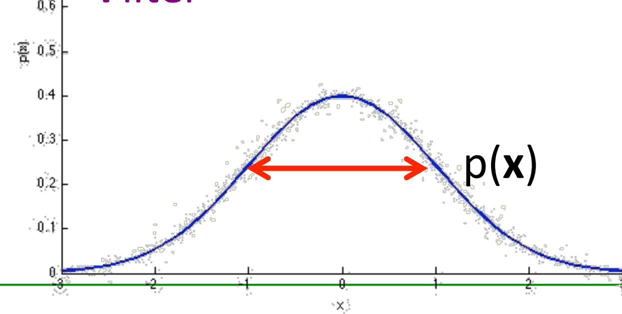


Sequential (KF) Approach:

Minimum Variance estimate

[minimum uncertainty]

- Optimal Interpolation (OI)
- (Extended / Ensemble) **K**alman **F**ilter



Courtesy: Kayo Ide

From Bayes theorem to 4DVar and the (Ensemble) Kalman Filter

$$p(\mathbf{x}|\mathbf{y}) \propto \exp\left(-(\mathbf{x}-\mathbf{x}_\mathrm{b})^\mathrm{T}\mathbf{P^b}^{-1}(\mathbf{x}-\mathbf{x}_\mathrm{b}) - (\mathbf{y}-\mathbf{Hx})^\mathrm{T}\mathbf{R}^{-1}(\mathbf{y}-\mathbf{Hx})\right)$$

Variational methods maximize the posterior PDF to find the state trajectory **x** that best fits the obs **y** in a least-squares sense. In practice, this is done by minimizing a cost function, which is what's inside the *exp*:

$$J(\mathbf{x}) \propto (\mathbf{x}-\mathbf{x}_\mathrm{b})^\mathrm{T}\mathbf{P^b}^{-1}(\mathbf{x}-\mathbf{x}_\mathrm{b}) + (\mathbf{y}-\mathbf{Hx})^\mathrm{T}\mathbf{R}^{-1}(\mathbf{y}-\mathbf{Hx})$$

The minimum can be found analytically if **H** is linear (see Lorenc 1986)
This gives the equations for the Kalman Filter

$$\boxed{\begin{gathered}\mathbf{x}_\mathrm{a} = \mathbf{x}_\mathrm{b} + \mathbf{K}\left(\mathbf{y}-\mathbf{H}\mathbf{x}_\mathrm{b}\right),\ \mathbf{P}^\mathrm{a} = \left(\mathbf{I}-\mathbf{KH}\right)\mathbf{P}^\mathrm{b} \\ \mathbf{K} = \mathbf{P}^\mathrm{b}\mathbf{H}^\mathrm{T}\left(\mathbf{H}\mathbf{P}^\mathrm{b}\mathbf{H}^\mathrm{T}+\mathbf{R}\right)^{-1}\end{gathered}}$$

- *Matrix* $\mathbf{P}^\mathrm{b}$ *is too big for any computer, covariance update step impractical.*
- *Instead, represent PDFs of* **x** *and* **y** *by an ensemble, compute sample estimate of* $\mathbf{P}^\mathrm{b}$ *and* $\mathbf{x}_\mathrm{b}$*. Evolve the sample, not the full covariance.* ***EnKF*** *gives same result as full KF if ensemble size becomes infinite.*

Computational shortcuts in EnKF:
(1) Simplifying Kalman gain calculation

$$\mathbf{K} = \mathbf{P}^{\mathrm{b}} H^{\mathrm{T}} \left(H\mathbf{P}^{\mathrm{b}} H^{\mathrm{T}} + \mathbf{R} \right)^{-1}$$

$$\text{define} \quad \overline{H\mathbf{x}^{\mathrm{b}}} = \frac{1}{m} \sum_{i=1}^{m} H\mathbf{x}_{\mathrm{i}}^{\mathrm{b}}$$

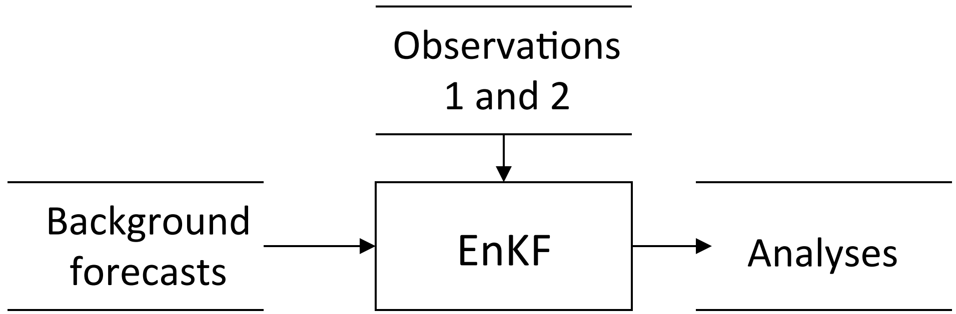
$$\mathbf{P}^{\mathrm{b}} H^{\mathrm{T}} = \frac{1}{m-1} \sum_{i=1}^{m} \left(\mathbf{x}_{\mathrm{i}}^{\mathrm{b}} - \overline{\mathbf{x}^{\mathrm{b}}} \right) \left(H\mathbf{x}_{\mathrm{i}}^{\mathrm{b}} - \overline{H\mathbf{x}^{\mathrm{b}}} \right)^{\mathrm{T}}$$

$$H\mathbf{P}^{\mathrm{b}} H^{\mathrm{T}} = \frac{1}{m-1} \sum_{i=1}^{m} \left(H\mathbf{x}_{\mathrm{i}}^{\mathrm{b}} - \overline{H\mathbf{x}^{\mathrm{b}}} \right) \left(H\mathbf{x}_{\mathrm{i}}^{\mathrm{b}} - \overline{H\mathbf{x}^{\mathrm{b}}} \right)^{\mathrm{T}}$$

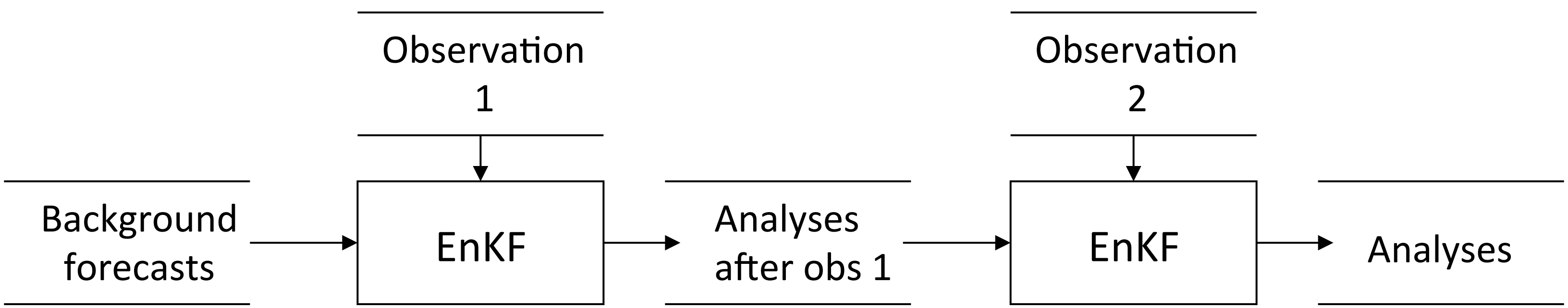
The key here is that the huge matrix $\mathbf{P}^{\mathrm{b}}$ is never explicitly formed

Computational shortcuts in EnKF: (2) serial processing of observations (requires observation error covariance **R** to be diagonal)

Method 1



Method 2



The serial EnKF – a recipe

Given a single ob y^o with expected error variance R, an ensemble of model forecasts $\mathbf{x}^b$ (model priors), and an ensemble of predicted observations $\mathbf{y}^b = \mathbf{H}\mathbf{x}^b$ (observation priors):

Step 1: Update observation priors.

(1a) $\overline{\mathbf{y}}_\mathrm{a} = (1-\mathrm{K})\overline{\mathbf{y}}_\mathrm{b} + \mathrm{K}\mathrm{y}^\mathrm{o}$ *update for ob prior means*

(1b) $\mathbf{y}_\mathrm{a}^{'} = \sqrt{(1-\mathrm{K})}\mathbf{y}_\mathrm{b}^{'}$ *rescaling of ob prior perturbations*

where the scalar K = var($\mathbf{y}^b$)/(var($\mathbf{y}^b$)+ R), overbar denotes means, prime denotes perturbations, superscript *b* denotes prior, *a* denotes analysis.

Linear interpolation between observation and observation prior mean *with weight K (0<=K<=1), rescaling of observation prior ensemble so posterior variance is consistent with Kalman filter, i.e.* var($\mathbf{y}^a$)=(1-K) var($\mathbf{y}^b$)= var($\mathbf{y}^b$)R/(var($\mathbf{y}^b$)+R).

when var($\mathbf{y}^b$) << R, all weight given to prior.

when var($\mathbf{y}^b$) >> R, all weight given to observation.

The serial EnKF – a recipe (2)

Step 2: Update model priors.

Let $\Delta\mathbf{x} = \mathbf{x}^a - \mathbf{x}^b$ be analysis increment for model priors, $\Delta\mathbf{y} = \mathbf{y}^a - \mathbf{y}^b$ is analysis increment for observation priors.

(2) $\Delta\mathbf{x} = \mathbf{G}\Delta\mathbf{y}$ *computation of increments to model prior*

where $\mathbf{G} = \mathrm{cov}(\mathbf{x}^b, \mathbf{y}^{bT})/\mathrm{var}(\mathbf{y}^b)$

Linear regression of model priors on observation priors.

Only changes model priors when $\mathbf{x}^b$ and $\mathbf{y}^b$ are correlated within the ensemble.

If there is more than one ob to be assimilated, the observation priors for other (not yet assimilated) obs ($\mathbf{Y}^b$) should be also be updated using (2) with $\Delta\mathbf{x}$ replaced by $\Delta\mathbf{Y}$. Next iteration, replace $\mathbf{y}^b$ with next column of $\mathbf{Y}^b$, removing that column from $\mathbf{Y}^b$. After each iteration the model priors and observation priors are set to the latest analysis values ($\mathbf{x}^a$ replaces $\mathbf{x}^b$, $\mathbf{Y}^a$ replaces $\mathbf{Y}^b$). Continue iterating until $\mathbf{Y}^b$ is empty.

Inflation and Localization

- **Inflation**
  – Used to inflate ensemble estimate of uncertainty to avoid filter divergence (additive and multiplicative)

- **Localization**
  – **Domain Localization**
    - Solves equations independently for each grid point (LETKF)
  – **Covariance Localization**
    - Performed element wise (Schur product) on covariances themselves

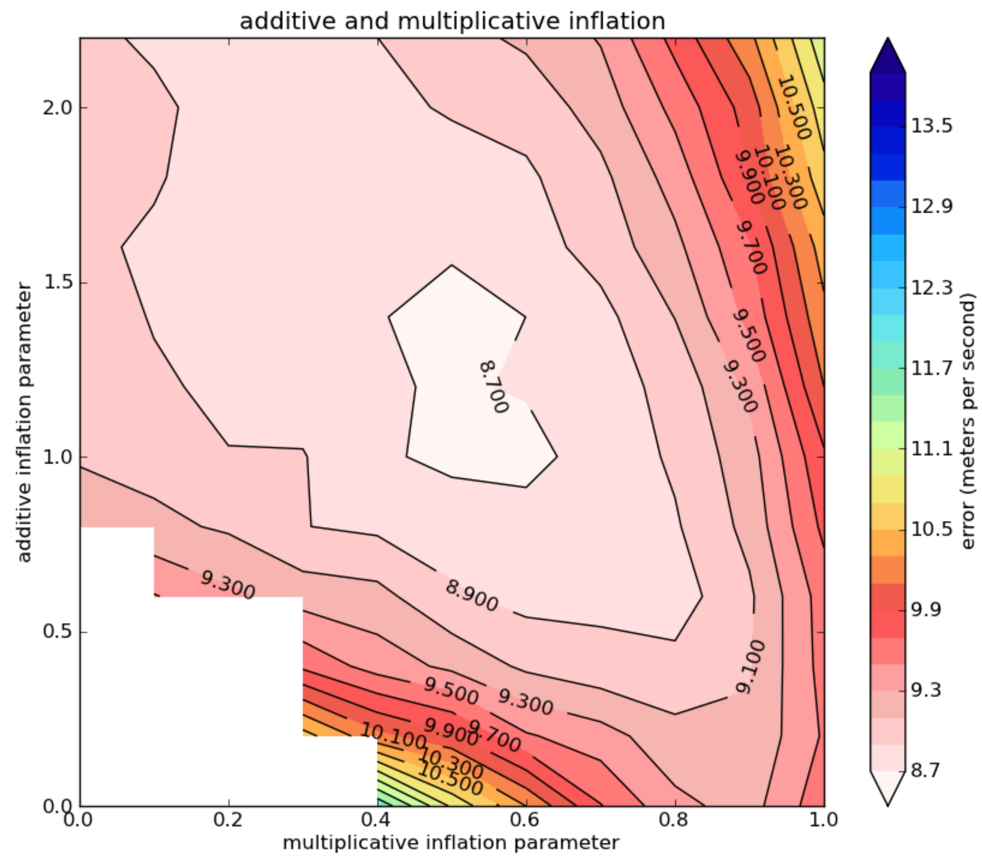
Methods for representing model error (inflation)

- **Multiplicative inflation**:
  - Relaxation-to-prior spread (RTPS) $\sigma^a \leftarrow (1-\alpha)\sigma^a + \alpha\sigma^b$
  - Relaxation-to-prior perturbation (Zhang et al. 2004)
  - Adaptive (Anderson 2007)

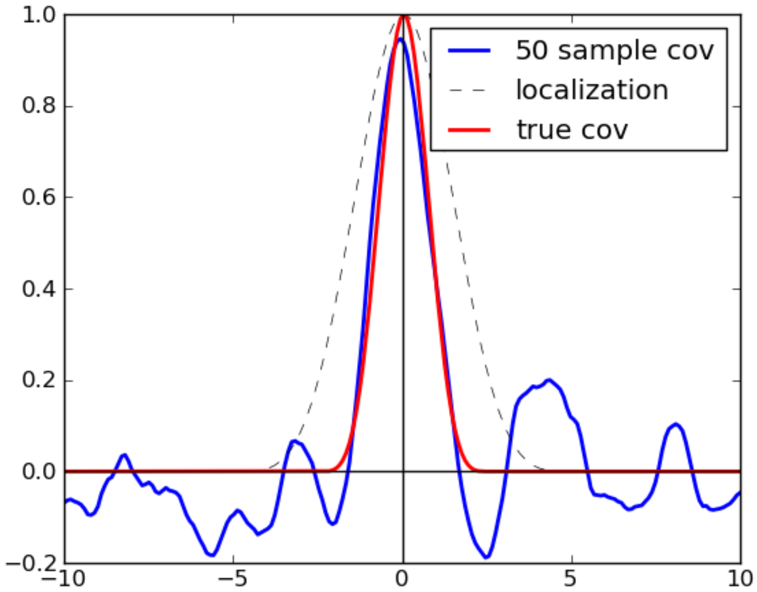
- **Additive inflation**: Add random samples from a specified distribution to each ensemble member after the analysis step.
  - Env. Canada uses random samples of isotropic 3DVar covariance matrix.
  - NCEP used random samples of 48-h – 24-h forecast error (fcsts valid at same time).

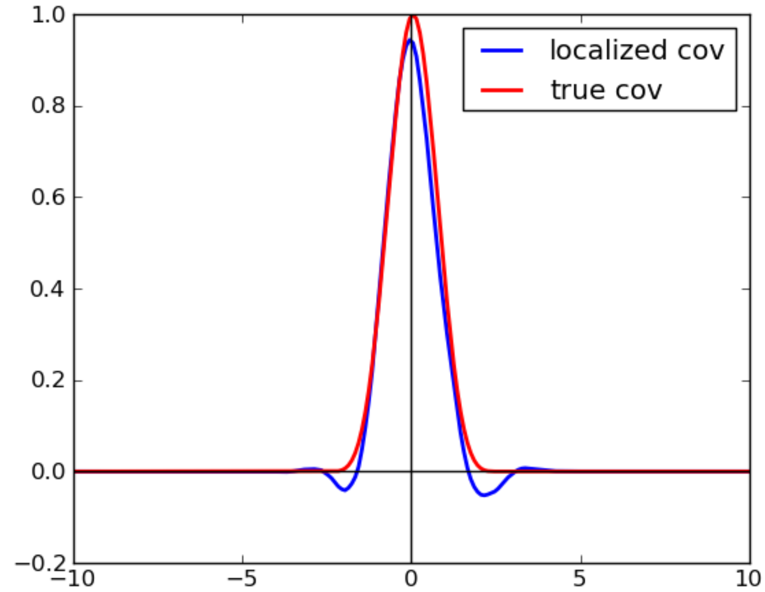
Imperfect Model (*Additive + Multiplicative Inflation Example)*

- Additive inflation alone outperforms multiplicative inflation alone (compare values y-axis to values along x-axis)
- A combination of both is better than either alone.
- Multiplicative and additive inflation representing different error sources in the DA cycle?



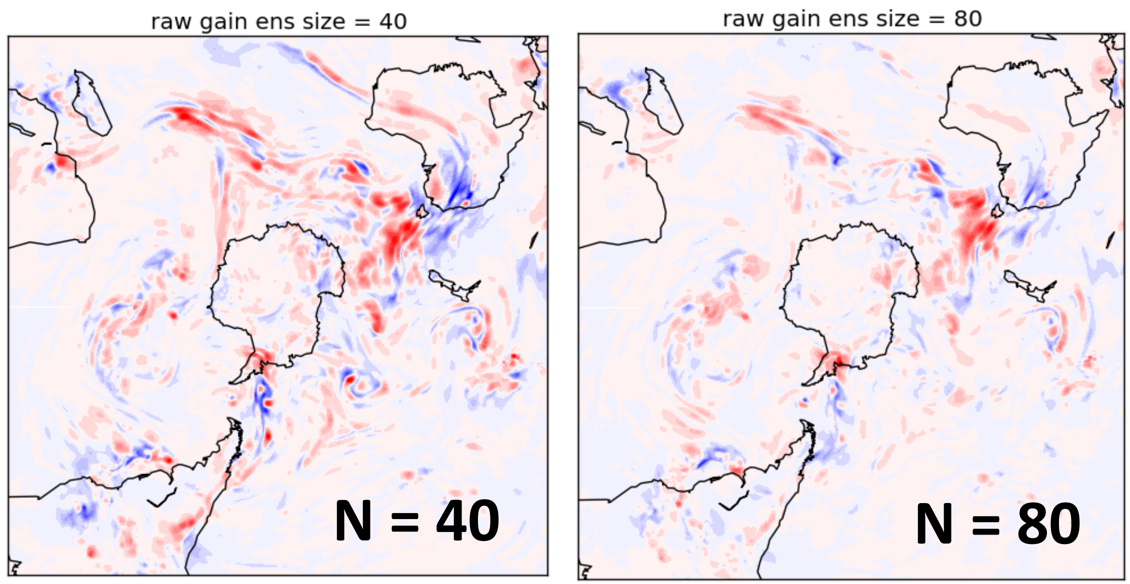
Covariance Localization – Simple Example



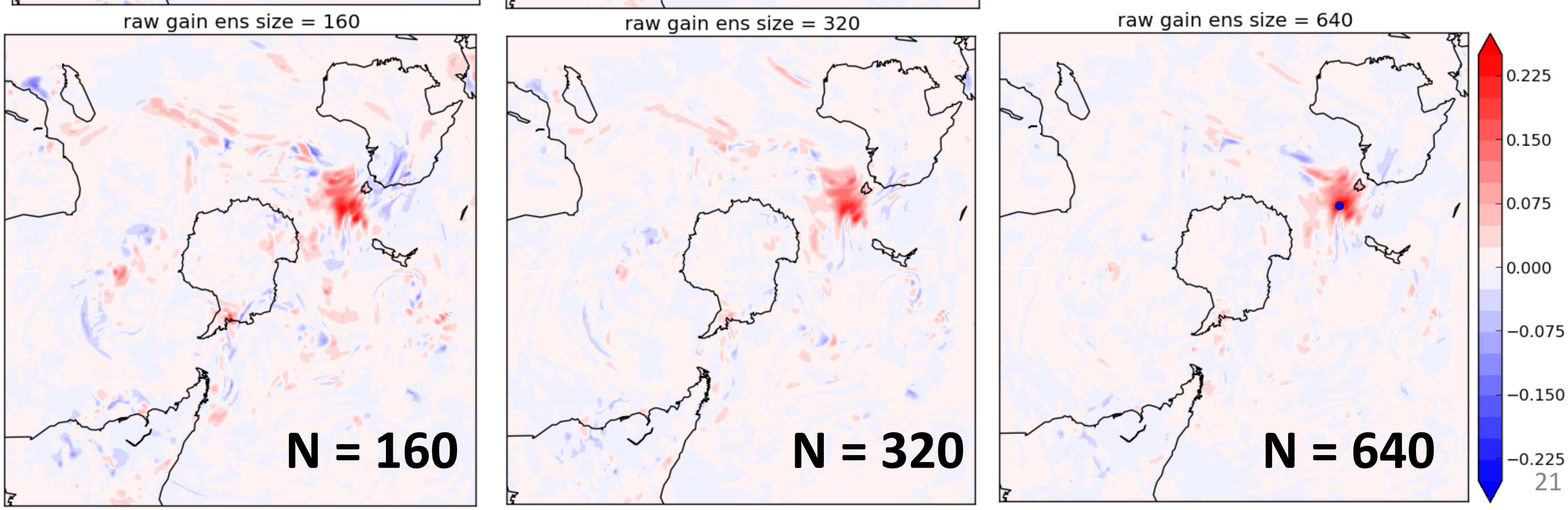


Estimates of covariances from a small ensemble will be noisy, with signal-to-noise small especially when covariance is small

Covariance localization – NWP Ex.



- AMSUA NOAA15 channel 6 radiance at 150E,-50S.
- Increment to level 30 (~310mb) temperature for a 1K O-F for 40, 80, 160, 320 and 640 ens members with no localization.



Factors limiting EnKF performance

1) Treatment of model error

Must account for the background error covariance associated with "model error" (any difference between simulated and true environment). Methods used so far:

1) multiplicative inflation (mult. ens perts by a factor > 1).
2) model-based schemes (e.g. stochastic kinetic energy backscatter for representing unresolved processes, stochastically perturbed physics tendecies for representing parameterization uncertainty).
3) additive inflation (random perts added to each member – e.g. differences between 24 and 48-h forecasts valid at the same time).

Operational NCEP system uses the first two.

Factors limiting EnKF performance

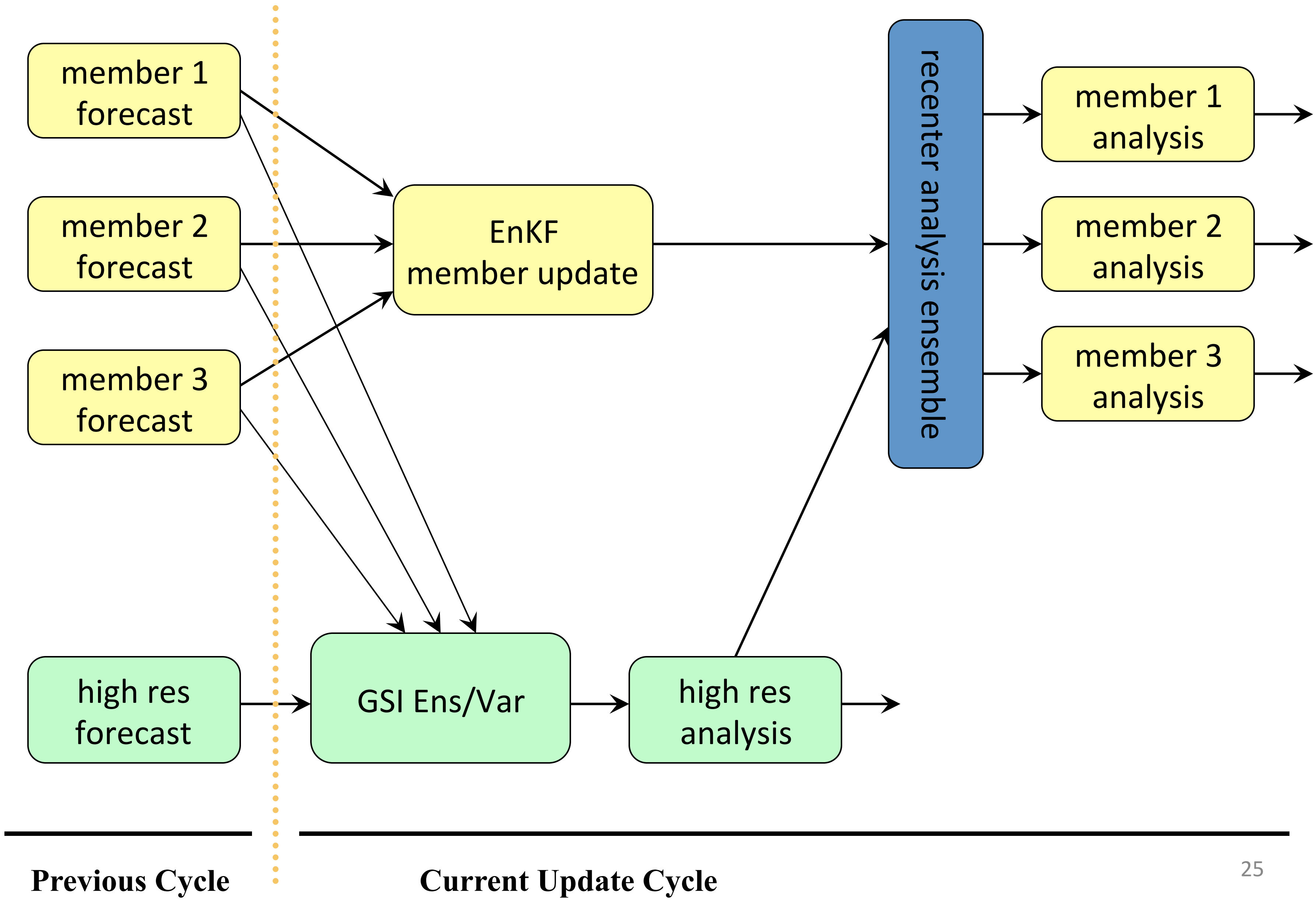
2) Treatment of sampling error (localization)

- All EnKF implementations localize the spatial impact of observations on the model state.
- Done by spatially modulating covariance between obs. prior and model state, or by only using observations 'close' to a model state variable to update that variable.
- Needed to account for low rank of ensemble (compared to model state).
- Methods used currently are not flow dependent, and assume there is no sampling error at ob location.

Why combine EnKF and Var?

Features from EnKF	Features from Var
Can propagate $\mathbf{P}^b$ from across assimilation windows	Treatment of sampling error in ensemble $\mathbf{P}^b$ estimate does not depend on $\mathbf{H}$.
More flexible treatment of model error (can be treated in ensemble)	Dual-resolution capability – can produce a high-res "control" analysis.
Automatic initialization of ensemble forecasts.	Ease of adding extra constraints to cost function, including a static $\mathbf{P}^b$ component.

Ensemble-Var workflow



Summary

- The EnKF uses an ensemble of first-guess forecasts to estimate the background-error covariance. Every ensemble member is updated at each analysis time.
  - Parallel code, scalable out to O(1000's) of processors as long as number of obs << number of state vars.
  - Requires state vector in model and ob space, plus obs, as input.
  - GSI used to compute forward observation operator (separate step run before EnKF).
- Need to carefully tune localization length scales (depends on model resolution, observing network).
- Ensemble (co)variances must be representative of control forecast error. Treatment of model error is crucial.