How 4DVAR can benefit from or contribute to EnKF (a 4DVAR perspective)

Dale Barker

WWRP/THORPEX Workshop on 4D-Var and Ensemble Kalman Filter Intercomparisons

Sociedad Cientifica Argentina, Buenos Aires, Argentina,
November 10-13th 2008

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Alternative Formulations of Advanced DA

- **Information/analysis space** analysis step (ECMWF, Met. Office, etc…):

$$\boldsymbol{x}^a - \boldsymbol{x}^b = \left[\mathbf{H}^T\mathbf{R}^{-1}\mathbf{H} + \mathbf{P_f}^{-1}\right]^{-1}\mathbf{H}^T\mathbf{R}^{-1}\left[\boldsymbol{y} - H(\boldsymbol{x}^b)\right]$$

- **Error/observation** space form (PSAS, NAVDAS, EnKF):

$$\boldsymbol{x}^a - \boldsymbol{x}^b = \mathbf{P_f}\mathbf{H}^T\left[\mathbf{H}\mathbf{P_f}\mathbf{H}^T + \mathbf{R}^{-1}\right]^{-1}\left[\boldsymbol{y} - H(\boldsymbol{x}^b)\right]$$

- Both can be written in terms of a "Kalman Gain" **K**

$$\boldsymbol{x}^a - \boldsymbol{x}^b = \mathbf{K}\left[\boldsymbol{y} - H(\boldsymbol{x}^b)\right]$$

- Equivalence between 4D-Var/EKF for Gaussian errors/linear model.

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4D-Var vs. EnKF (Kalnay et al 2007)

Table 7. Adaptation of the table of advantages and disadvantages of EnKF and 4-D-Var (Lorenc, 2003). Parentheses indicate disadvantages, square brackets indicate clarifications and italics indicate added comments

Advantages (disadvantages) of EnKF
Simple to design and code.
Does not need a smooth forecast model [i.e. model parametrizations can be discontinuous].
Does not need perturbation [linear tangent] forecast and adjoint models.
Generates [optimal] ensemble [initial perturbations that represent the analysis error covariance].
Complex observation operators, for example rain, coped with automatically, but sample is then fitted with a Gaussian.
Non-linear observation operators are possible within EnKF, for example, MLEF.
Covariances evolved indefinitely (only if represented in ensemble)
Underrepresentation should be helped by 'refreshing' the ensemble.
(Sampled covariance is noisy) and (can only fit N data)
Localization reduces the problem of long-distance sampling of the 'covariance of the day' and increases the ability to fit many observations.
Observation localization can be used with local filters.
Advantages (disadvantages) of 4-D-Var
[Can assimilate asynchronous observations]
4-DEnKF can also do it without the need for iterations. It can also assimilate time integrated observations such as accumulated rain.
Can extract information from tracers
4-DEnKF should do it just as well
Non-linear observation operators and non-Gaussian errors [can be] modelled
Maximum Likelihood Ensemble Filter allows for the use of non-linear operators and non-Gaussian errors can also be modelled.
Incremental 4-D-Var balance easy.
In EnKF balance is achieved without initialization for perfect models. For real observations, digital filtering may be needed.
Accurate modelling of time-covariances (but only within the 4-D-Var window)
Only if the background error covariance (not provided by 4-D-Var) includes the errors of the day, or if the assimilation window is long.

Kalnay vs. Gustaffson (2007)

"The data assimilation community is at a transition point, with a choice between variational methods…., and ensemble methods." *Kalnay et al. (2007a).*

"The idea of gradual development should..be applied to the ongoing discussions on 4D-Var and EnKF…More appropriate to ask "How can ideas from EnKF and 3/4D-Var best be combined"." *Gustaffson (2007).*

"Completely agree….Ideas developed in 4D-Var…can be easily adapted and included within EnKF". *Kalnay et al. (2007b)*

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Fundamental Issues (Covered this week)

- Balance (Errico, Polavarapu, Kepert, Fillion, …):
  - 4D-Var: Dynamical/statistical balance, Weak-constraint DF.
  - EnKF: Use balance constraint to correct localization effects.
  - Joint: Spin-up/initialization (especially at convective-scale).

- Nonlinearity/non-Gaussianity (Fisher, Yang, …):
  - 4D-Var: Outer-loop, variable transforms, VarQC.
  - EnKF: Adoption of outer-loop. MLEF approach.

- Model Error (Tremolet, Kalnay, …):
  - 4D-Var: Weak constraint 4D-Var. Equivalance with EKF.
  - EnKF: 'Particularly vulnerable'. Inflation + bias removal (e.g. Dee & DaSilva)

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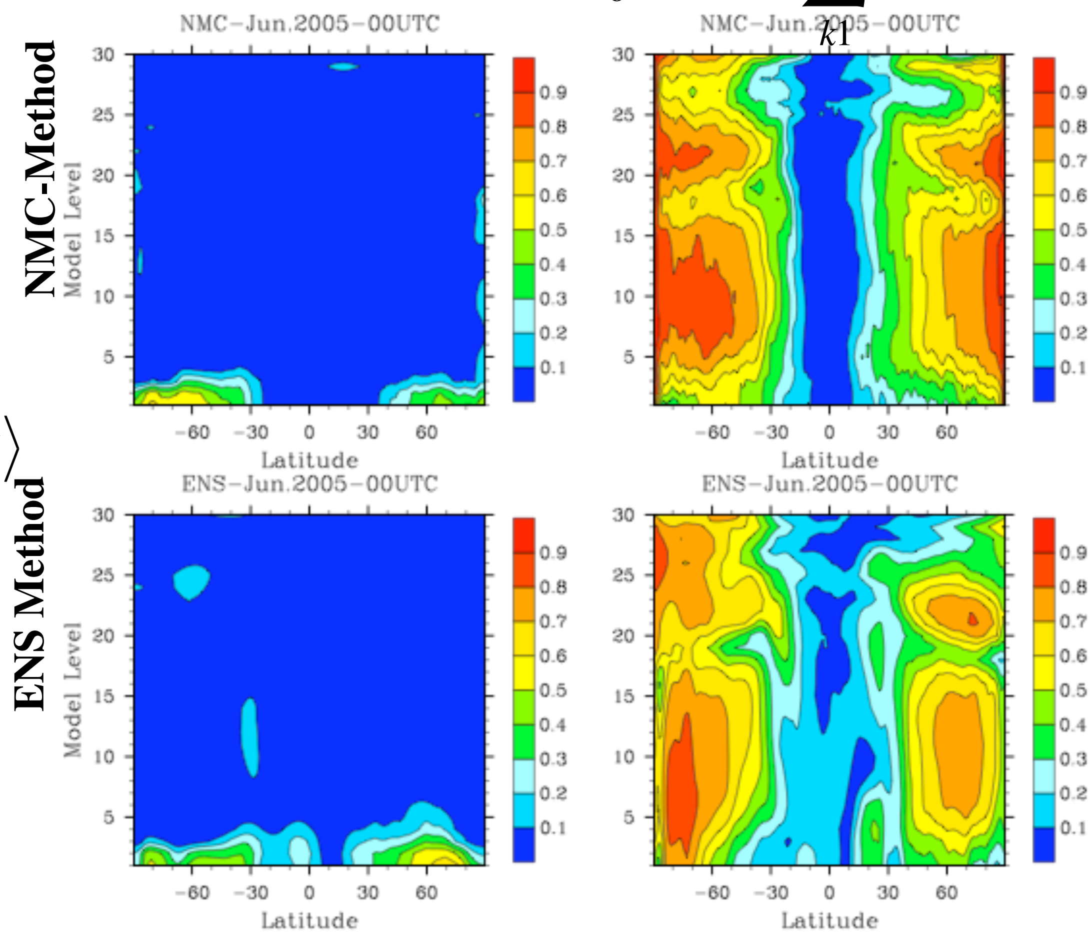
Ensemble/NMC-method based Climatological Statistical Balance

- T+48-T+24 fcst. Differences for NMC-method.
- T+12 KMA EPS (16 bred-mode) ensemble Data.
- June 2005 data.

$$\chi_b^{'} = c\,\psi^{'} \qquad T_b^{'}(k) = \sum_{k1} G(k,k1)\,\psi^{'}(k1)$$

$$\langle \chi_b \bullet \chi \rangle \langle \chi \bullet \chi \rangle \qquad \langle T_b \bullet T \rangle \langle T \bullet T \rangle$$



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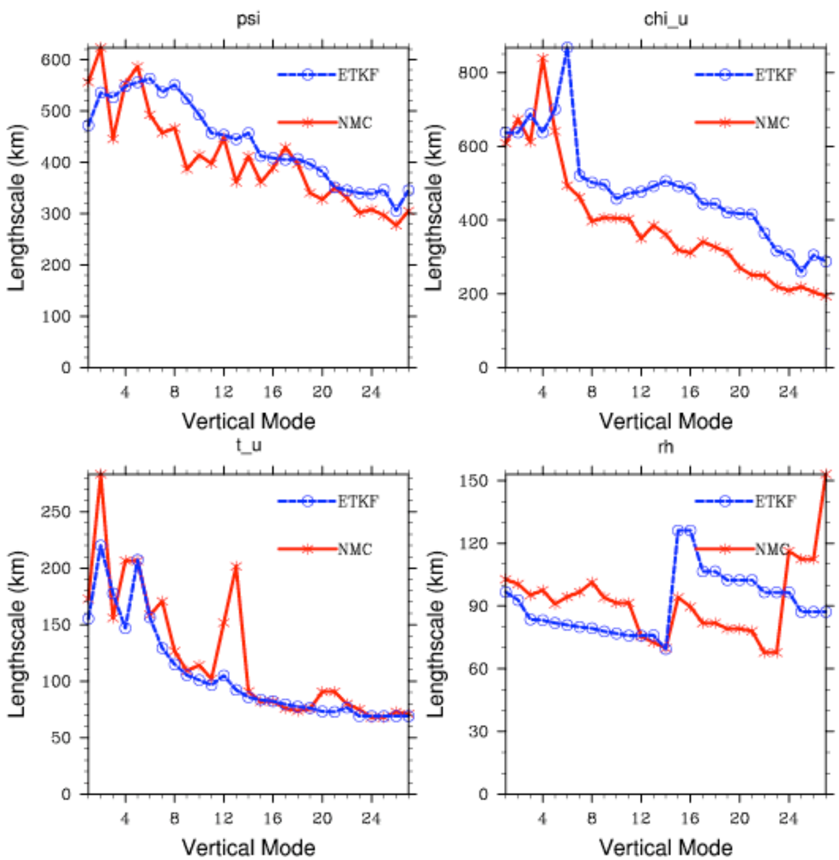
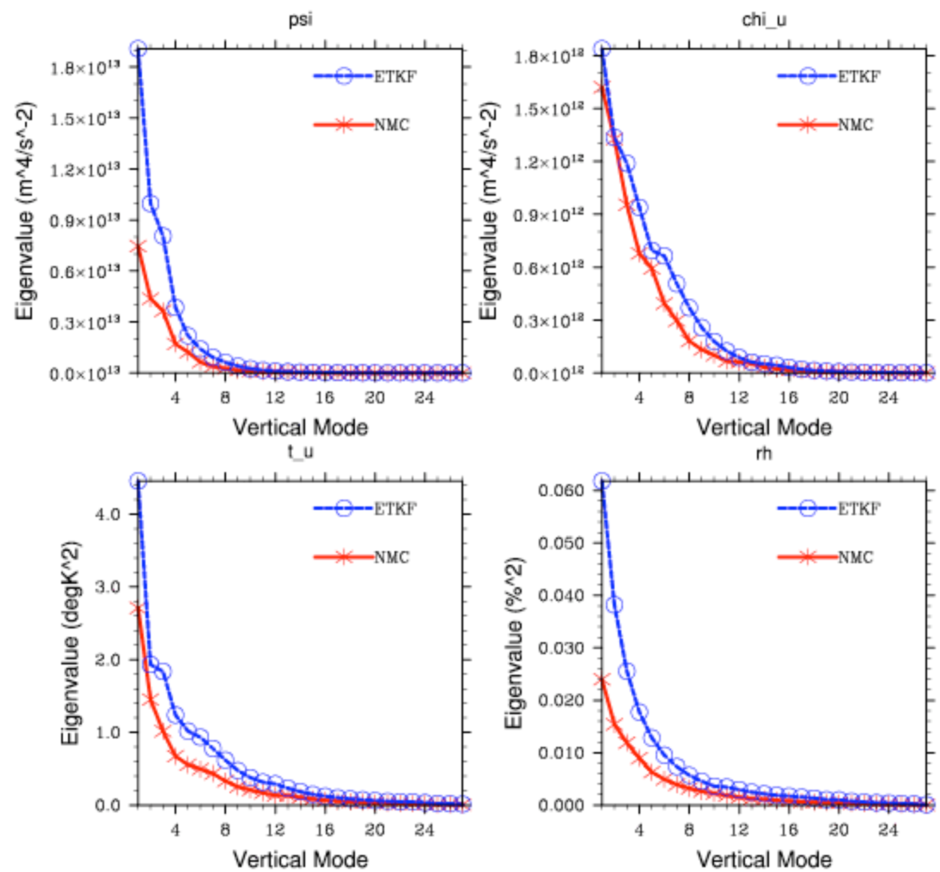
ETKF vs NMC-method Climatological Covariances (regional WRF)

Horizontal Correlation Scales



Eigenvalues (Variances)



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Positive Impact of ETKF-based covariances

(Wang, Barker,Hamill, and Snyder, 2008a)

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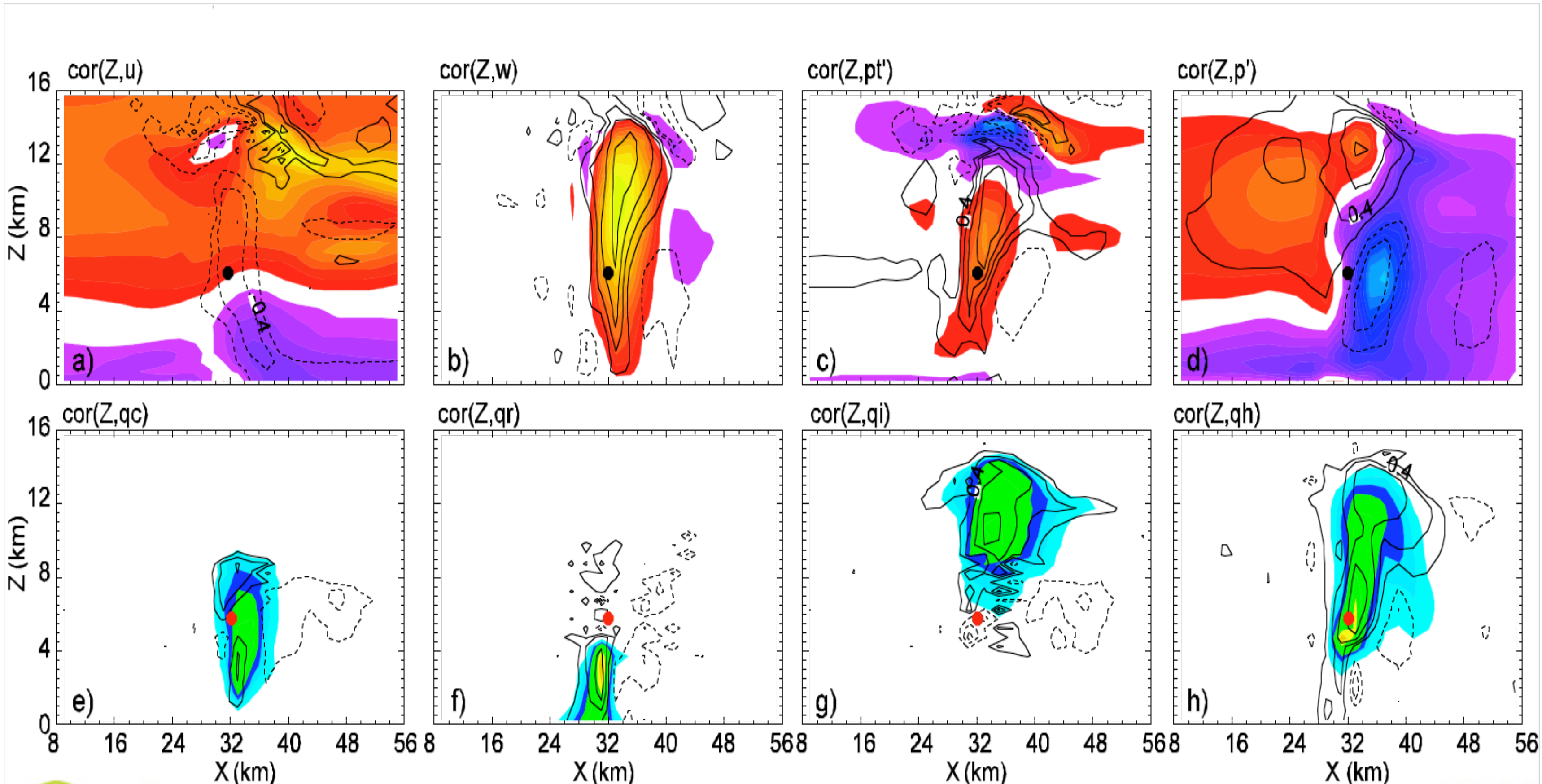
EnKF Convective-Scale Multivariate Forecast Error Covariances (Z=reflectivity) (Ming Xue)

Shading : True Fields **Line Contours : Error Correlations**



Study offline to train statistical balance in VAR?

Fundamental Issues (Covered this week)

- Balance (Errico, Polavarapu, Kepert, Fillion, …):
  - 4D-Var: Dynamical/statistical balance, Weak-constraint DF.
  - EnKF: Use balance constraint to correct localization effects.
  - Joint: Spin-up/initialization (especially at convective-scale).

- Nonlinearity/non-Gaussianity (Fisher, Yang, …):
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  - EnKF: Adoption of outer-loop. MLEF approach.

- Model Error (Tremolet, Kalnay, …):
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Maximum Likelihood Ensemble Filter (Zupanski 2005)

- A variational or an ensemble data assimilation scheme?

- Minimizes nonlinear 4D-Var cost function:

$$J = \frac{1}{2}\left(\mathbf{x}-\mathbf{x}_b\right)^{\mathbf{T}}\mathbf{P}_{\mathbf{f}}^{-1}\left(\mathbf{x}-\mathbf{x}_b\right)+\frac{1}{2}\left[\mathbf{y}^o - H(\mathbf{x})\right]^{\mathbf{T}}\mathbf{R}^{-1}\left[\mathbf{y}^o - H(\mathbf{x})\right]$$

- Hessian preconditioning via change of variable to minimize in ensemble space (using ensemble covariance $\mathbf{P_f}$):

$$\mathbf{x}-\mathbf{x}_b = \mathbf{P}_{\mathbf{f}}^{1/2}\left(\mathbf{I}+\mathbf{C}\right)^{-\mathbf{T}/2}\zeta$$

- Like the ETKF, cannot localize directly in ensemble space.

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Ensemble-Based 4D-Var 'En4DVAR' (Liu et al. 2008a,b)

- A variational or an ensemble data assimilation scheme?

- Define 'control variable transform' using ensemble perturbations

$$\delta \mathbf{x} = \delta \mathbf{X}_f \mathbf{w}$$

- Solves incremental, preconditioned 4D-Var cost function:

$$J(\mathbf{w}) = \frac{1}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} + \frac{1}{2}\sum_{i=0}^{I}\left[\mathbf{HM}\delta\mathbf{X}_{\mathbf{f}}\mathbf{w} + \mathbf{d}_{\mathbf{i}}\right]^{\mathrm{T}}\mathbf{R}_i^{-1}\left[\mathbf{HM}\delta\mathbf{X}_{\mathbf{f}}\mathbf{w} + \mathbf{d}_{\mathbf{i}}\right]$$

- Gradient calculation uses ensembles rather than adjoint model:

$$\nabla_w J = \mathbf{w} + \sum_{i=0}^{I}\mathbf{U}^{\mathrm{T}}\mathbf{M}^{\mathrm{T}}\mathbf{H}^{\mathrm{T}}\mathbf{R}_i^{-1}\left[\mathbf{HMUw} + \mathbf{d}_{\mathbf{i}}\right]$$

$$\nabla_w J = \mathbf{w} + \sum_{i=0}\left[\mathbf{HM}\delta\mathbf{X}_{\mathbf{f}}\right]^{\mathrm{T}}\mathbf{R}_i^{-1}\left[\mathbf{HM}\delta\mathbf{X}_{\mathbf{f}}\mathbf{w} + \mathbf{d}_{\mathbf{i}}\right]$$

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Fundamental Issues (Covered this week)

- Background Error Estimation (Berre, Hamill, Bishop, …):
  - 4D-Var: Full-rank $\mathbf{P_f}$. Flow-dependence modelled/via linear model.
  - EnKF: Sampling errors. Flow-dependent, based on nonlinear model. Adaptive localization.

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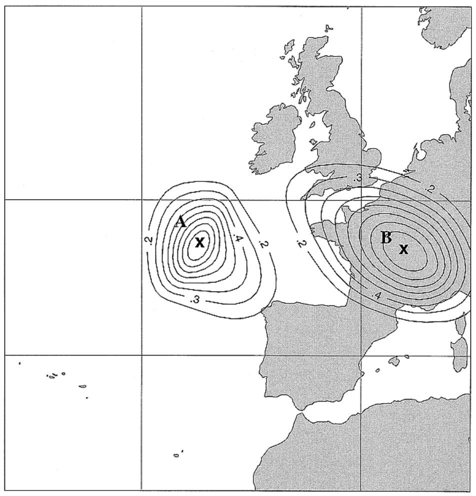
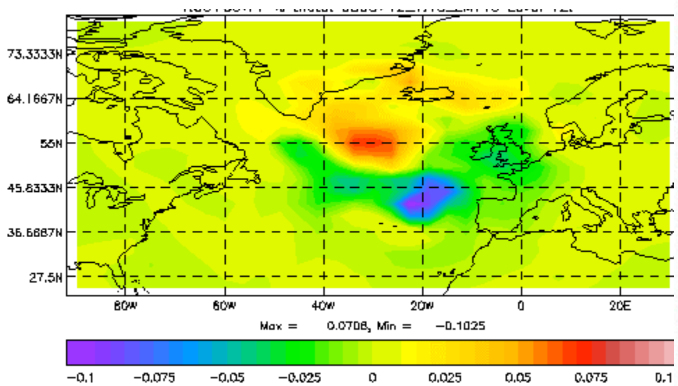
Flow-Dependent Forecast Errors in Var: Early Attempts

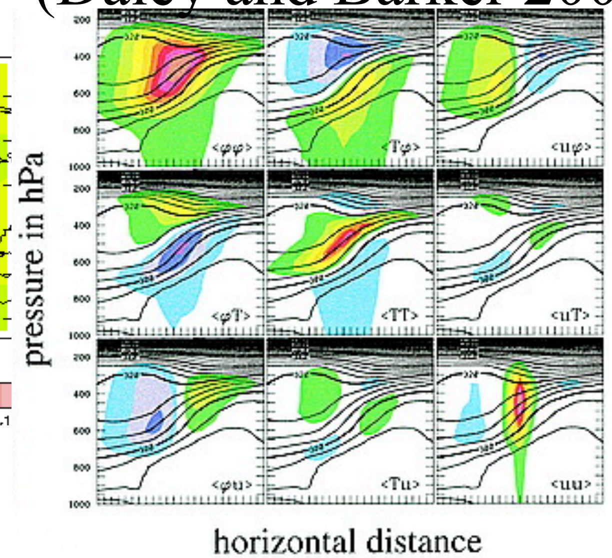
Desroziers (1997)



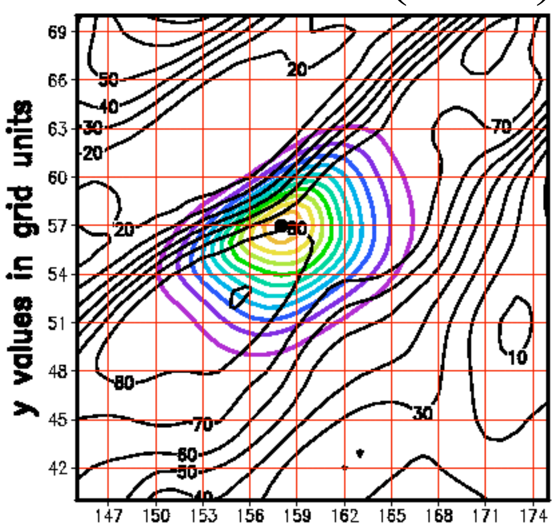
Barker (1999)



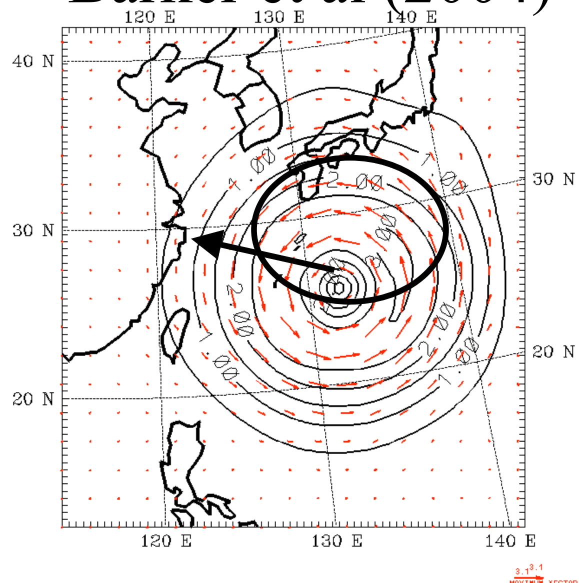
(Daley and Barker 2000)



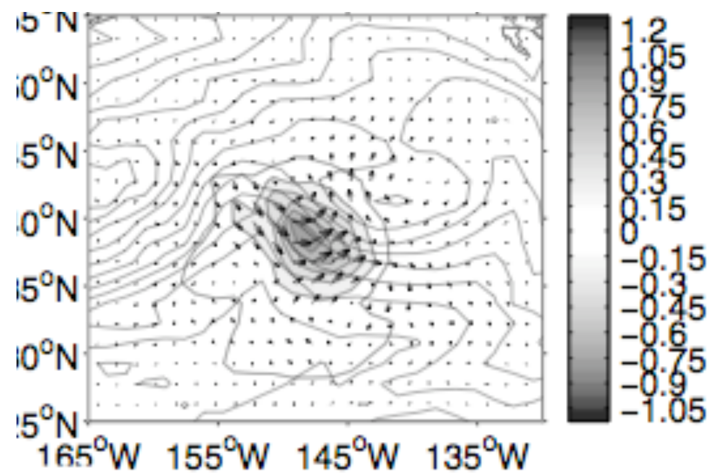
Purser et al (2003)



Barker et al (2004)



Buehner (2005)



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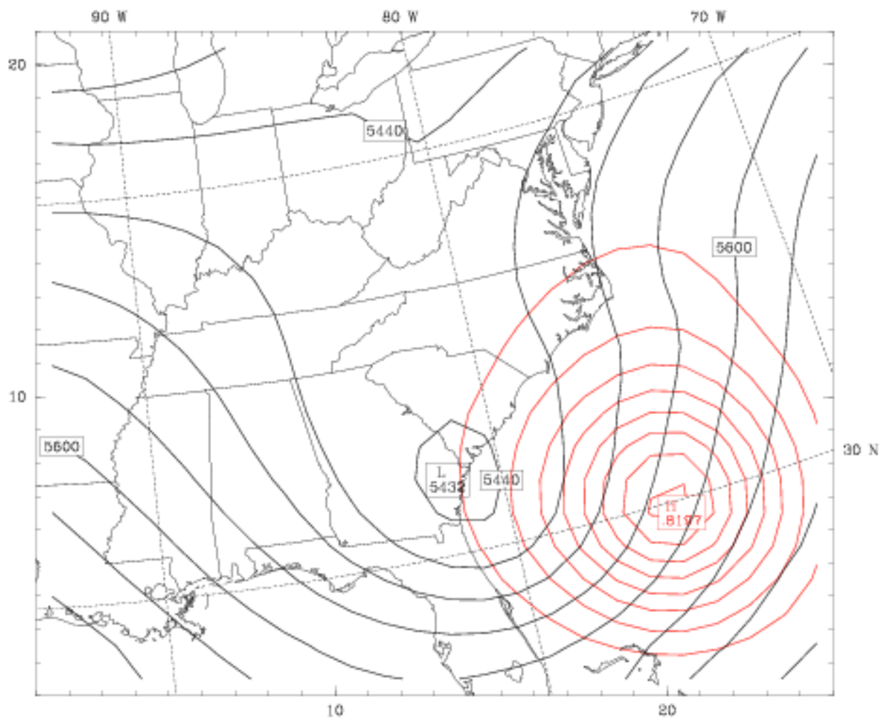
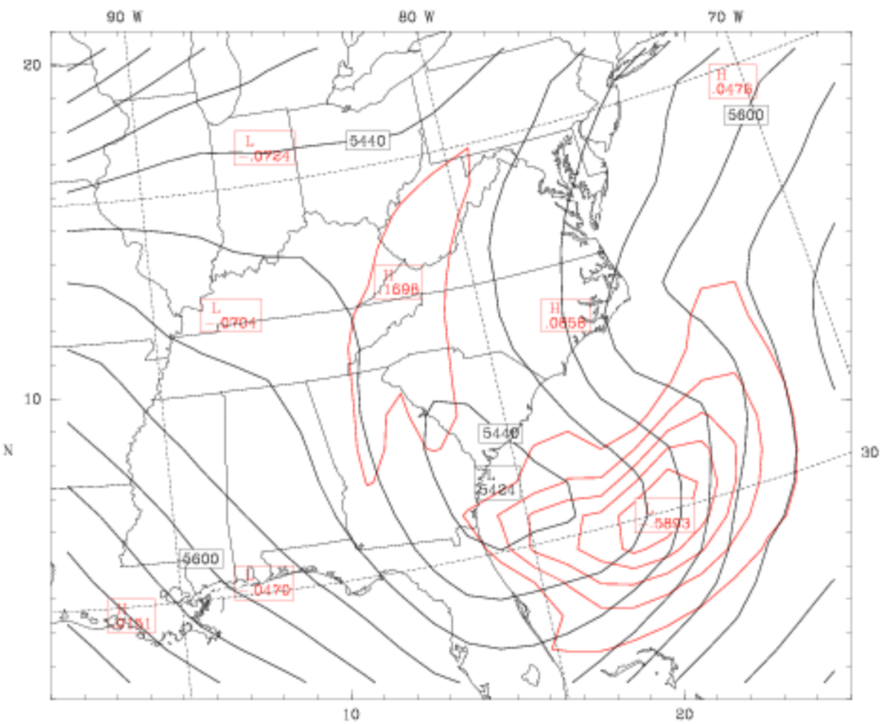
500mb θ increments from 3D-Var at 00h and from 4D-Var at 06h due to a 500mb T observation at 06h



3D-Var (NoFGAT)



4D-Var

(Hans Huang)

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Hybrid Variational/Ensemble DA

Benefits for Var:

- Introduces flow-dependent initial PDF in 3/4D-Var.
- Explicit coupling between moisture/temp/wind fields (tropics, high-res).
- Easily incorporated in Var framework.
- Relatively cheap (if properly preconditioned and compressed).
- Can't do worse – can switch off ensemble covariances if detrimental.
- Flow-dependent QC.

Benefits over ensemble filters:

- Hybrids more robust for small ensemble sizes and large model error.
- Cost does not scale with observations.
- Can couple with nonlinear QC (serial filter can't do that by itself).
- Ensemble used for covariance modeling only - can still run high-res mean.

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Hybrid Var/Ensemble DA References

- Barker (1999): Demonstration with 1 bred-mode + UKMO 3D-Var.
- Hamill and Snyder (2000): Hybrid in Ensemble Framework.
- Etherton and Bishop (2004): QG model.
- Buehner (2005): Additional control variable/3D-Var: Small impact.
- Wang, Hamill, Whitaker and Bishop (2007): Compare EnSRF/Hybrid/OI.
- Wang, Barker, Hamill and Snyder (2008a, b): WRF AlphaCV+3D-Var.

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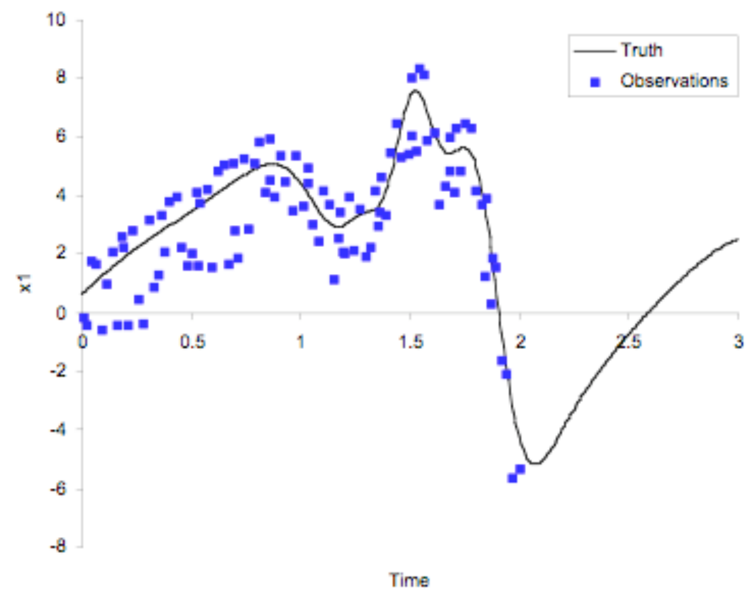
Hybrid Testing With Lorenz 1996 model (K. Y. Chung: KMA Visitor to NCAR)

$$\frac{d\mathbf{x}_i}{dt} = \left(\mathbf{x}_{i+1} - \mathbf{x}_{i-2}\right)\mathbf{x}_{i-1} - \mathbf{x}_i + \mathbf{F}$$



- 40-variable model (i=1, 40). **F**=8.
- Periodic boundary conditions $\mathbf{x}_1 = \mathbf{x}_\mathrm{I}$
- OSSE: dt=6h. Simulate obs every 12h. 400d run, verify last 200d.
- Hybrid 3D-Var/EnKF (Hamill and Snyder 2000): $\mathbf{P}^f = (1-\beta)\mathbf{P}_e^f + \beta\mathbf{B}_0$
- Flow-dependence $\mathbf{P}_e^f$ via a) Lagged forecast diff., b) EnKF perturbations.

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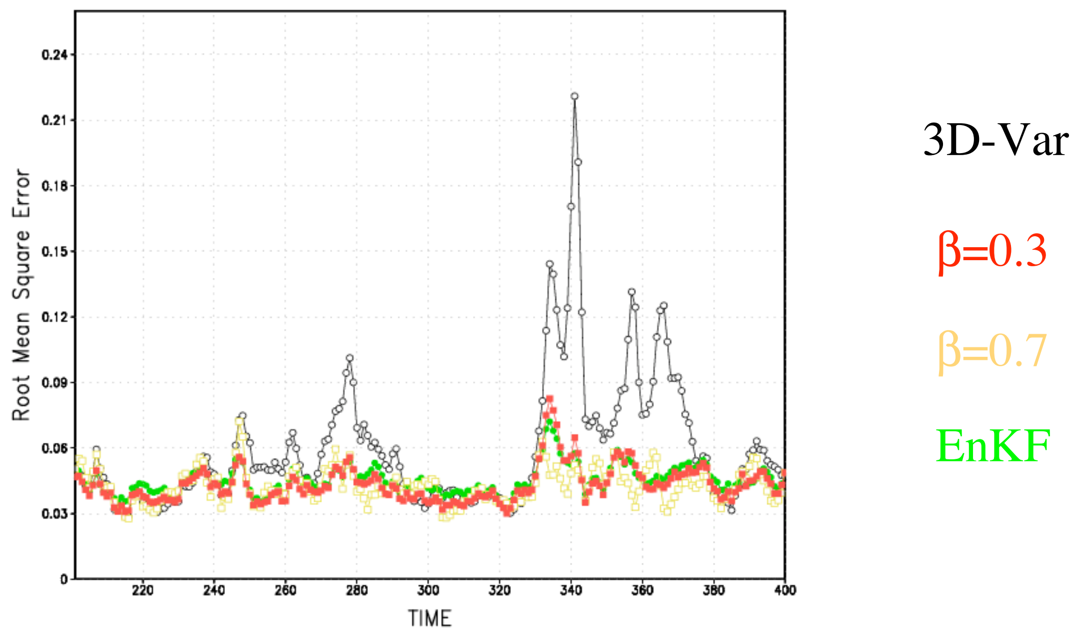
Lorenz Model OSSE Analysis Error, N=10

Root Mean Square Analysis Error (x100)

β	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
3D-Var	5.70								
Hybrid	4.21	4.33	**4.19**	4.46	4.32	4.37	4.86	5.00	5.20
EnSRF	4.59								



Example Hybrid Result
(Etherton and Bishop 2004)

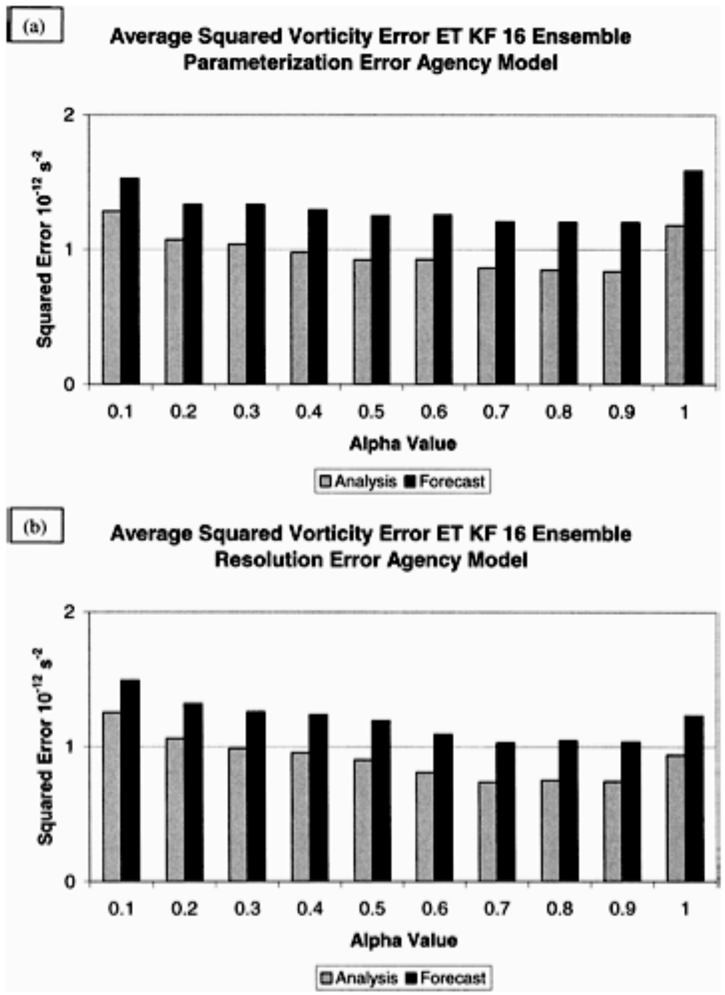


FIG. 5. The daily average squared vorticity error as a function of the parameter alpha ($\alpha = 0$ being pure ETKF, $\alpha = 1$ being pure 3DVAR) for when the agency's forecast model had (a) parameterization error or (b) resolution error. A 16-member ETKF-generated ensemble was used for the construction of the flow-dependent error statistics.

- Barotropic vorticity model.
- ETKF not localized.
- 3D (not 4D)-Var.
- Optimal mix of Var/Ens covariance ~70/30%.

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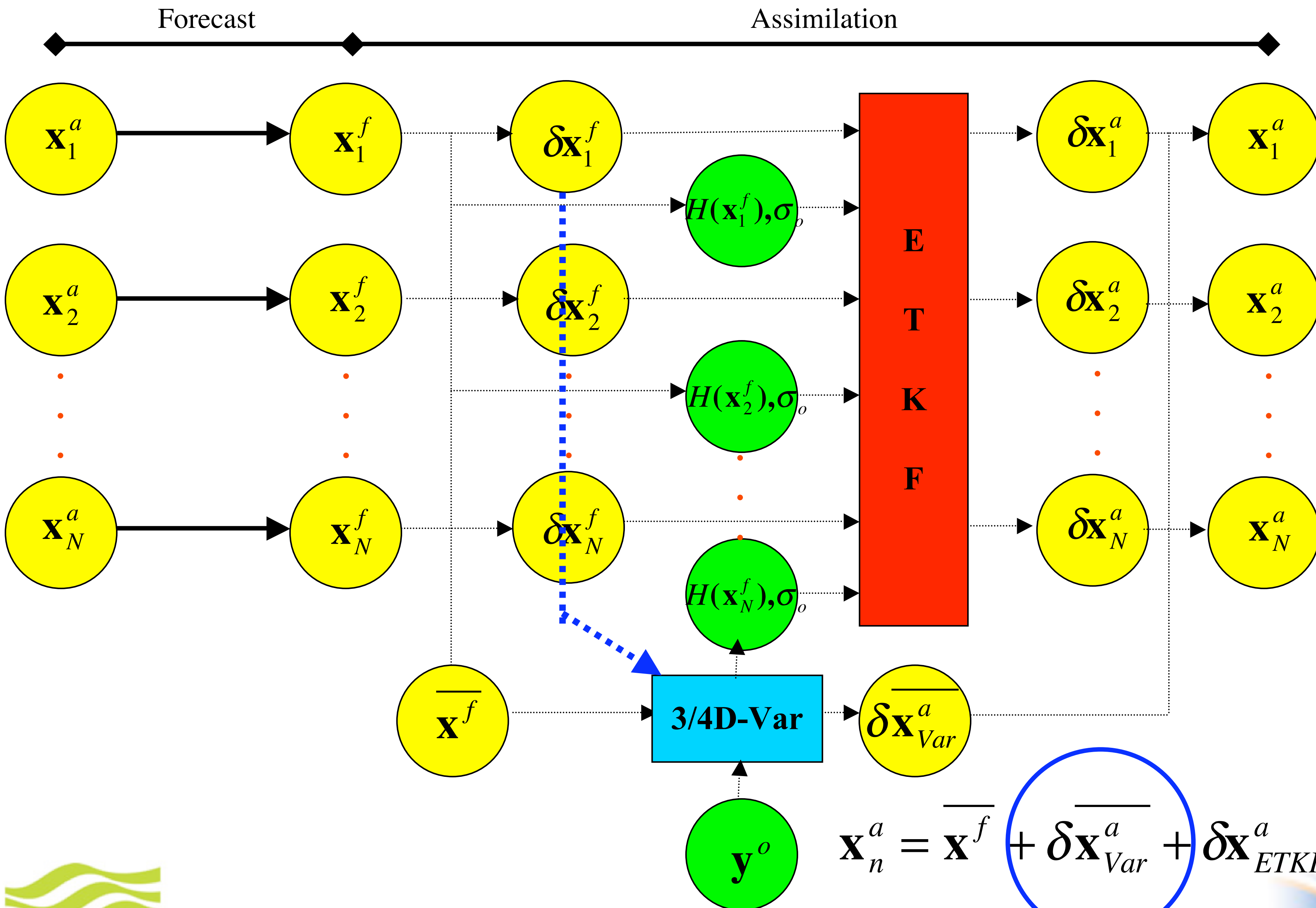
Cycling WRF/WRF-Var/ETKF System (Hybrid DA)



$$\mathbf{x}_n^a = \overline{\mathbf{x}^f} + \overline{\delta\mathbf{x}^a_{Var}} + \delta\mathbf{x}^a_{ETKFn}$$

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Hybrid DA Via Additional Control Variables

- Define the matrix of ensemble perturbations as

$$\delta\mathbf{X}_f = \left(\delta\mathbf{x}_{f1}, \delta\mathbf{x}_{f2}, \ldots, \delta\mathbf{x}_{fN}\right) \tag{1}$$

- Hybrid 3/4D-Var analysis increments give by

$$\delta\mathbf{x}_0 = \delta\mathbf{x}_{0d} + \delta\mathbf{X}_f \bullet \mathbf{a} = \mathbf{U}\mathbf{v} + \delta\mathbf{X}_f \bullet \mathbf{a} \tag{2}$$

- Note flow-dependence $\delta\mathbf{X}_f$ constrained by a new set of control variables

$$\mathbf{a}^{\mathrm{T}} = \left(\alpha_1, \alpha_2, \ldots, \alpha_N\right) \tag{3}$$

- Could alternatively define the hybrid in control variable space, e.g.

$$\delta\psi_0 = \delta\psi_{0d} + \delta\psi_f \bullet \mathbf{a} \qquad \delta\chi_{u0} = \delta\chi_{u0d} + \delta\chi_{uf} \bullet \mathbf{a} \tag{4}$$

- (4) better than (2) when balance well known (ref. Kepert).

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Cost Functions and Variance Conservation

- Flow-dependence is constrained by an additional cost-function J_α, i.e.

$$J = \frac{W_b}{2}\delta\mathbf{x}_0{}^T\mathbf{B}_o^{-1}\delta\mathbf{x}_0 + \boxed{\frac{W_\alpha}{2}\mathbf{a}^T\mathbf{A}^{-1}\mathbf{a}} + \frac{1}{2}\sum_{i=0}^{n}\left[\mathbf{H}_i\delta\mathbf{x}(t_i) - \mathbf{d}_i\right]^T\mathbf{R}_i^{-1}\left[\mathbf{H}_i\delta\mathbf{x}(t_i) - \mathbf{d}_i\right]$$

- Define empirical alpha covariance matrix $\mathbf{A} = \sigma_\alpha^2\mathbf{A}_c$

- W_b and W_α are weights defined to conserve forecast error.

- Lorenc (2003)-type hybrid conservation: $\frac{1}{\sqrt{W_b}} + \frac{1}{\sqrt{(W_\alpha/\sigma_\alpha^2)}} = 1$

- Forecast error variance conservation: $\frac{1}{W_b} + \frac{1}{W_\alpha/\sigma_\alpha^2} = 1$

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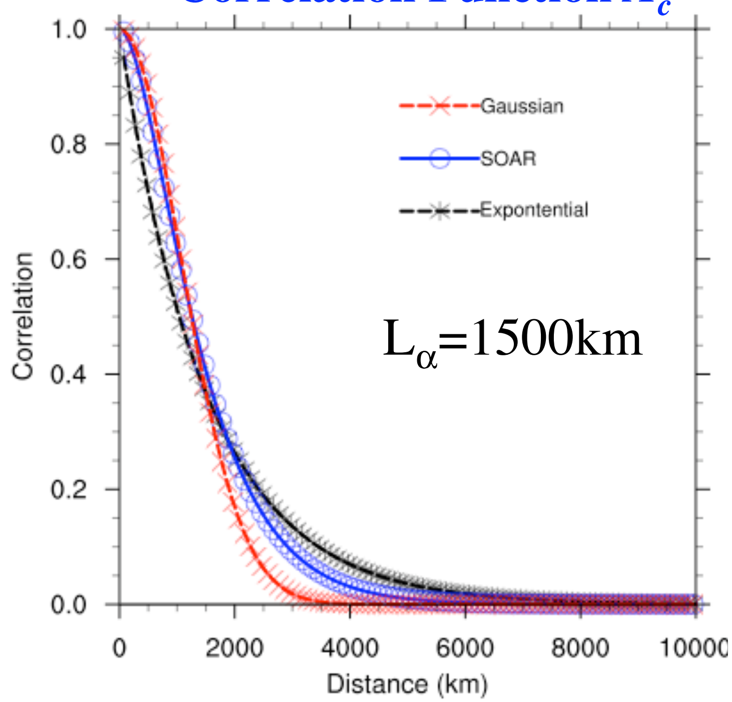
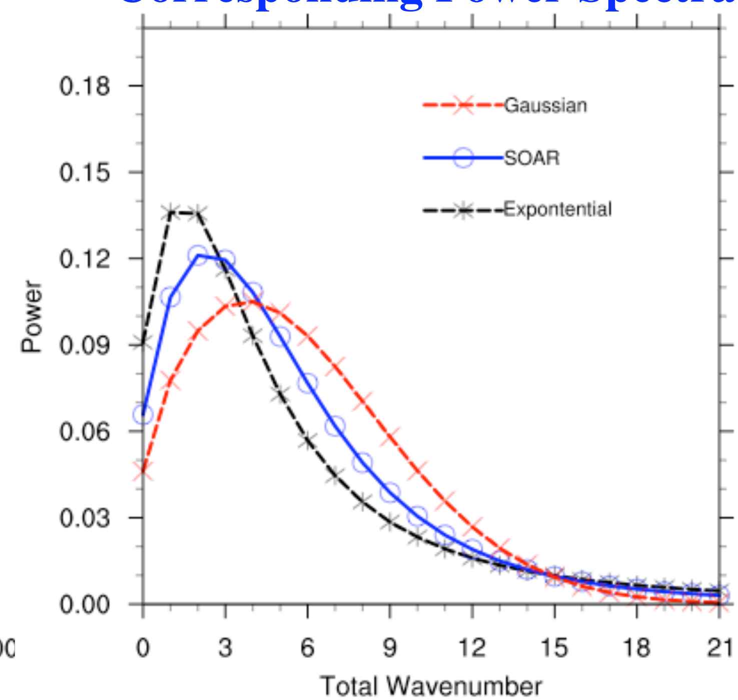
Example Application of ACV in Global WRF-Var

- Alpha correlation A_c is empirical function (e.g. Gaussian) with prescribed scale L_α.
- Lorenc (2003) suggest equivalence between A_c and covariance localization.
- Test ACV approach in global WRF-Var (spectral localization)

Correlation Function A_c



Corresponding Power Spectra



Practical vertical localization possible via similar data compression

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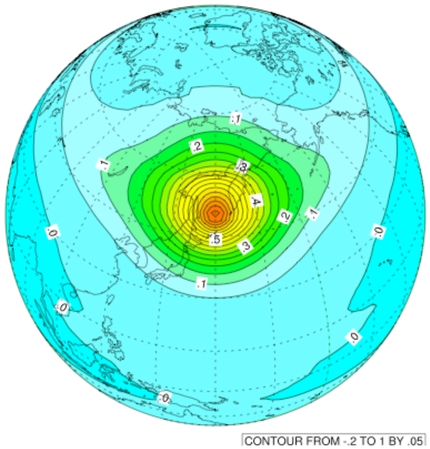
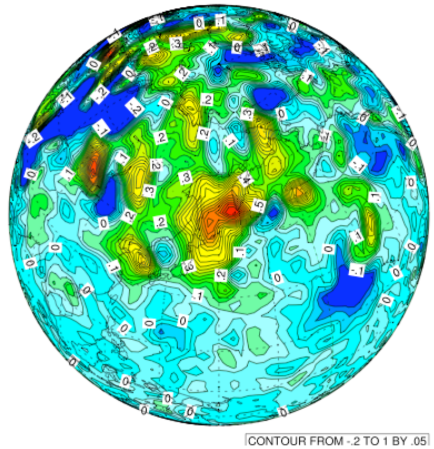
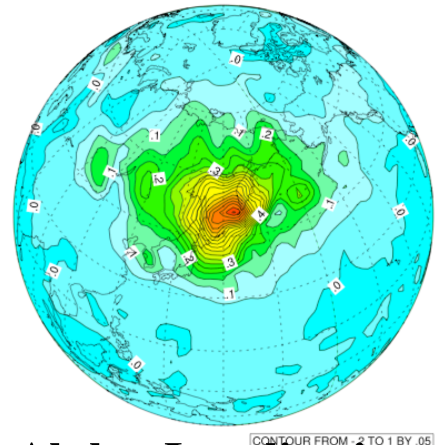
Single Observation Test - Alpha CV

- Specify single T observation (O-B, σ_o=1K) at 50N, 150E, 500hPa.
- Example: Flow-Dependence given by 1 member of KMA's EPS.

T' increment

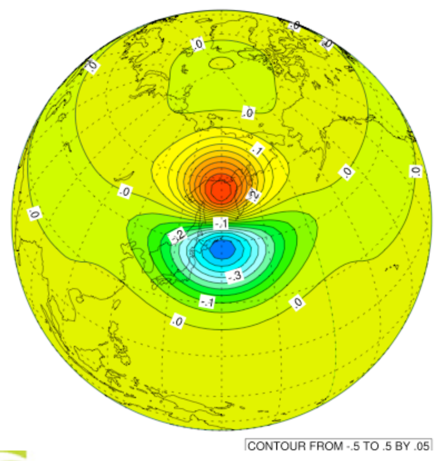


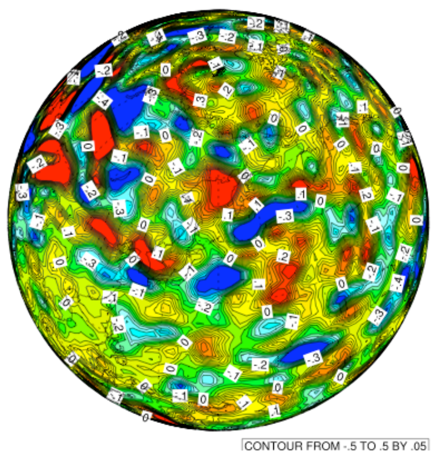


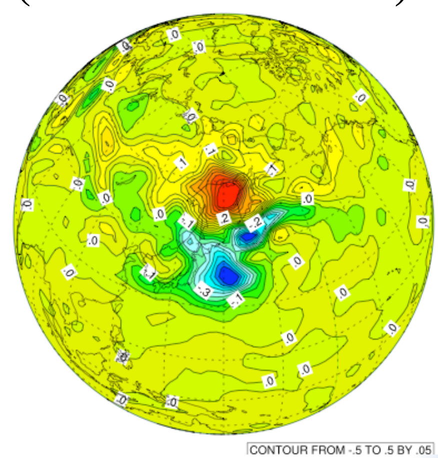


No Alpha | **Alpha, No Localization** | **Alpha, Localization (1500km Gaussian)**

u' increment







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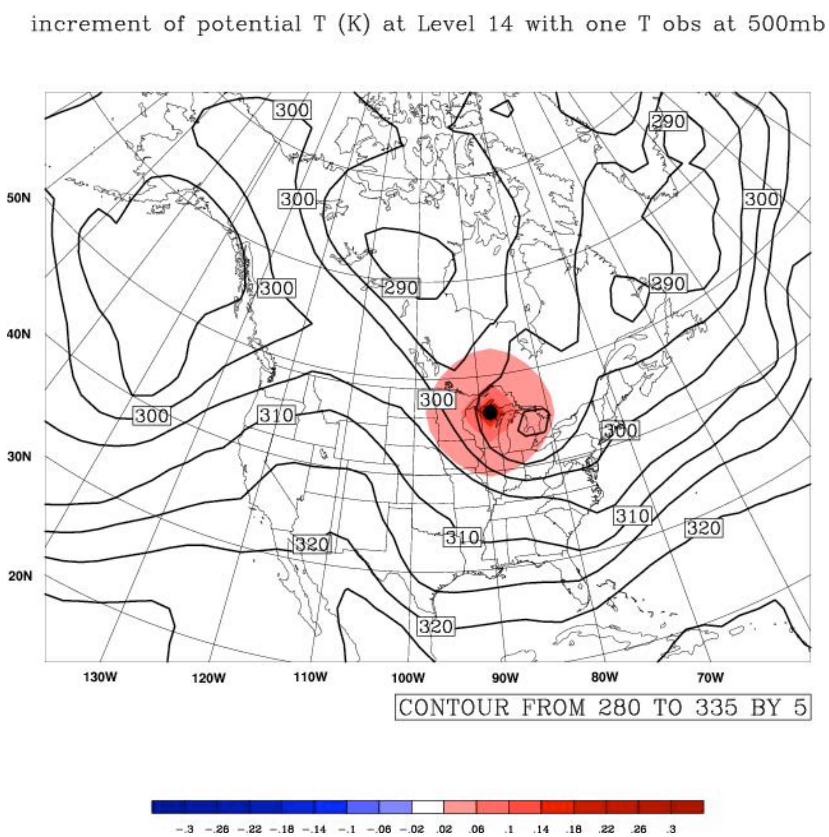
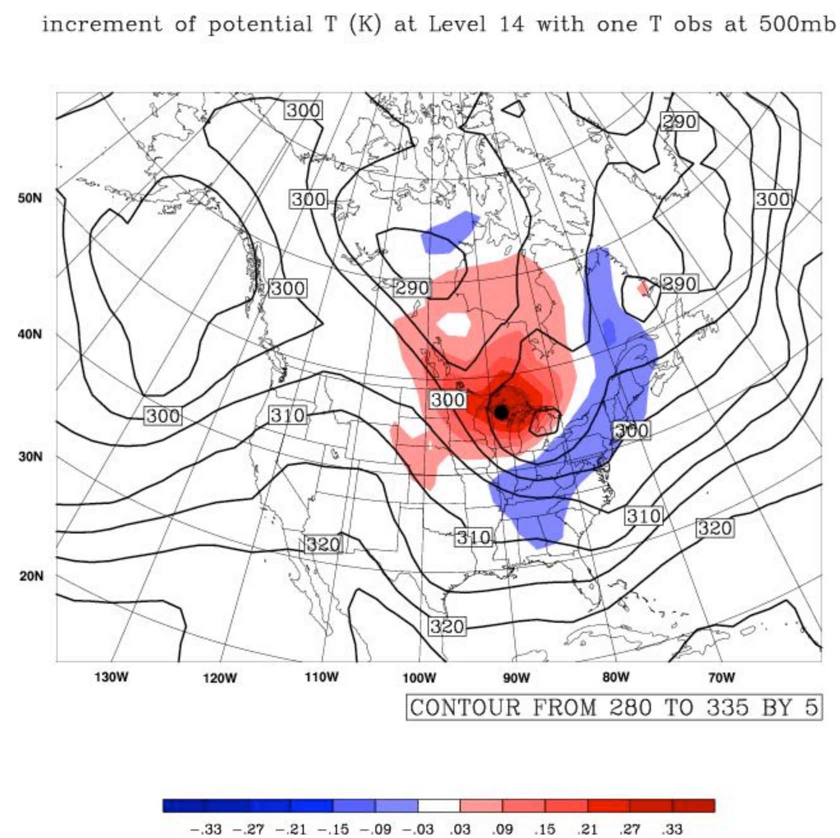
WRF Test with single observation (X. Wang)

Analysis increment

Static covariance



Ensemble covariance with localization



Flow-dependent ETKF ensemble covariance is successfully incorporated in WRF-Var

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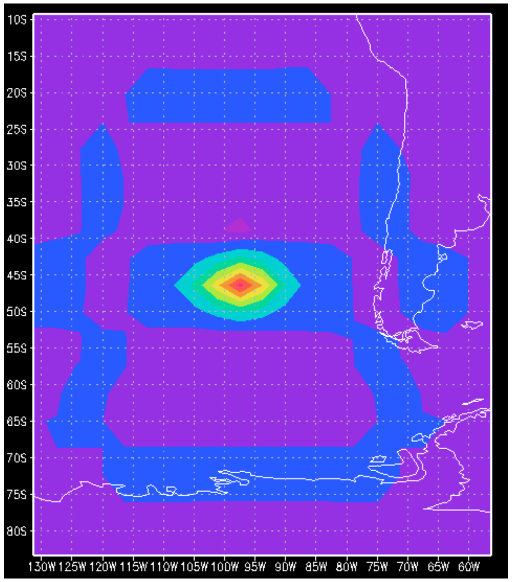
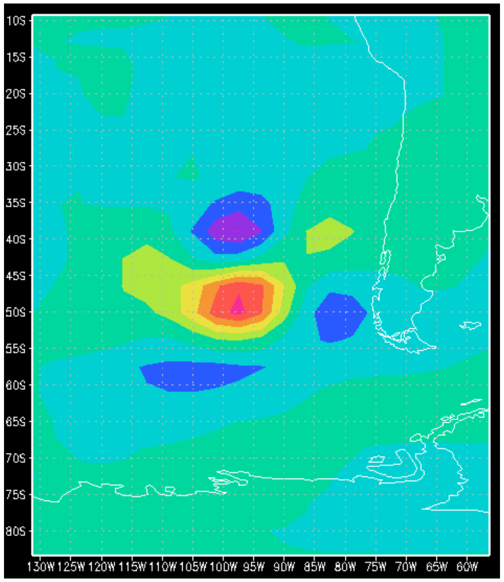
Hybrid In SPEEDY Model
(Incomplete, but I promised Eugenia!)

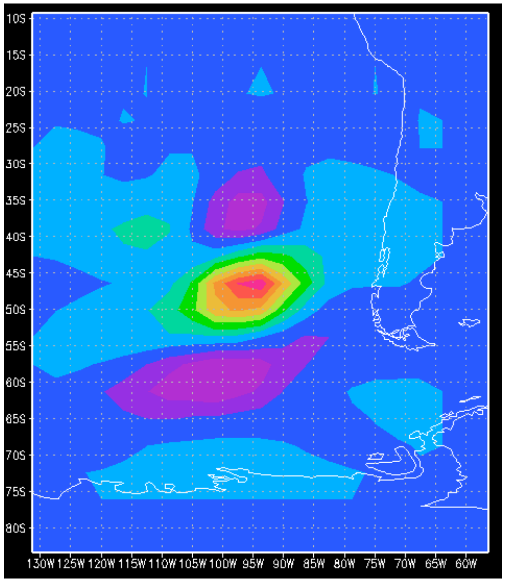
3DVAR



Hybrid (W_a=2)



LETKF



- Single u observation
- Hybrid equal weight on Var/ENS covariances.
- 1000km localization applied in hybrid.

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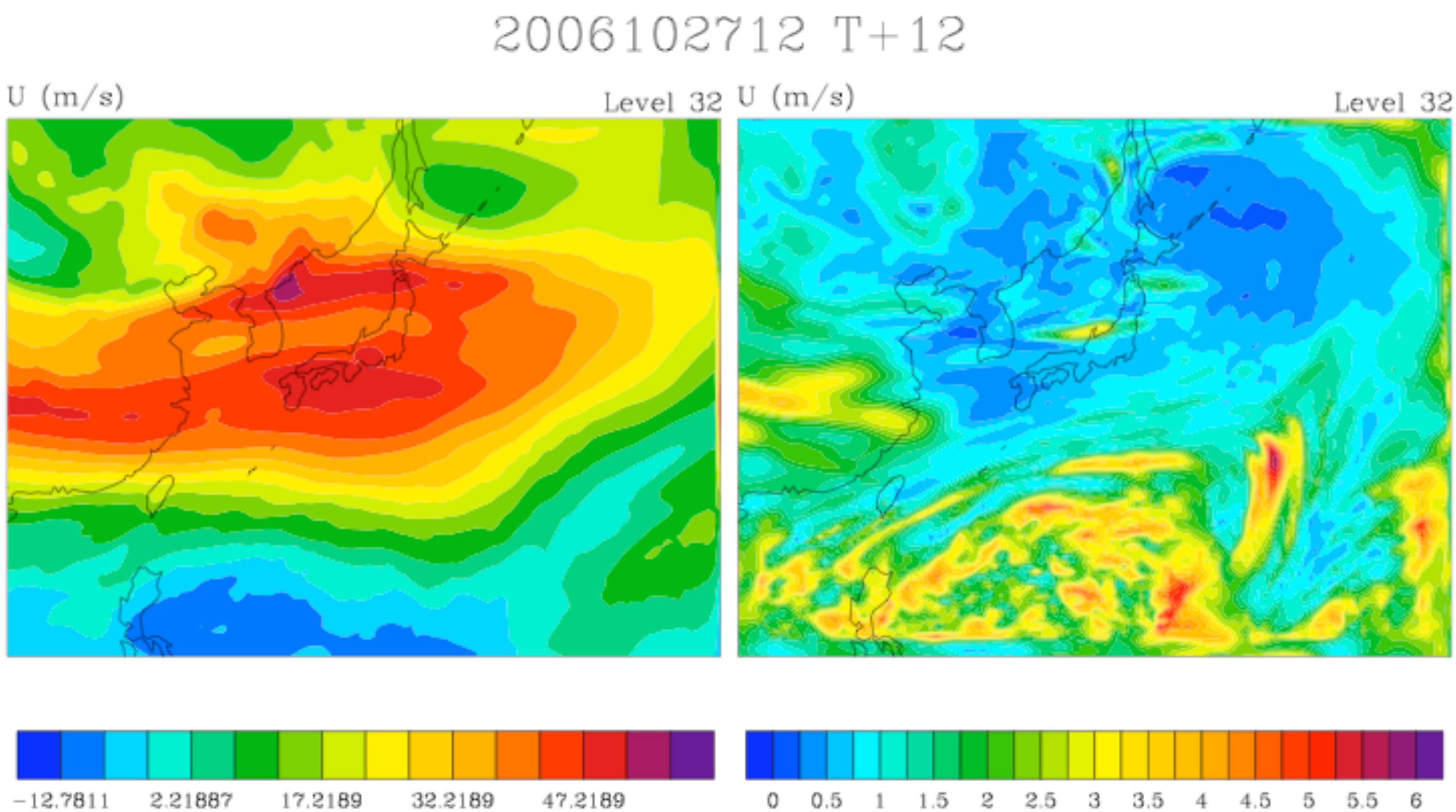
Regional WRF Application
(E. Asia, US Air Force, 10 members)



U Mean

U Spread

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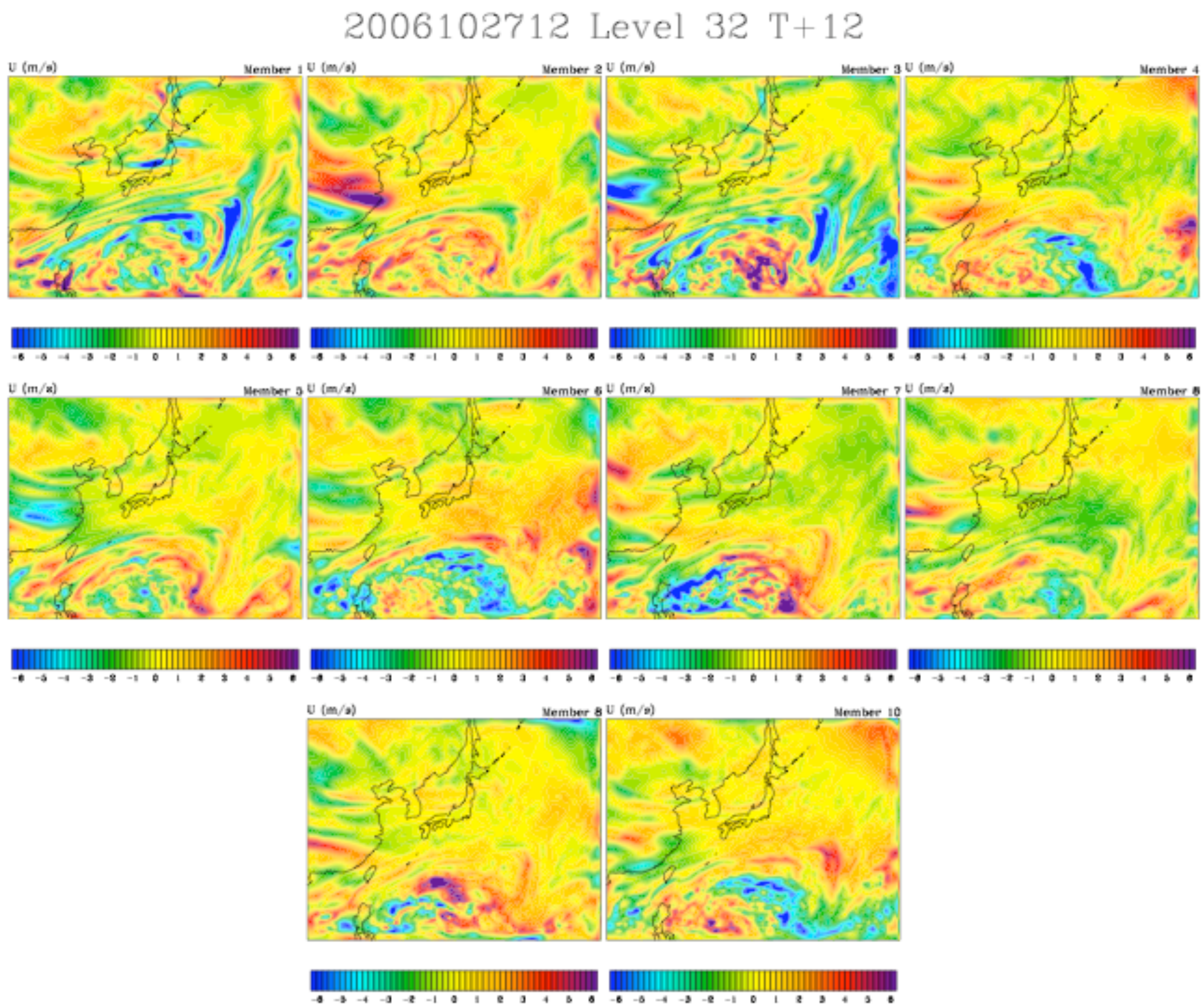
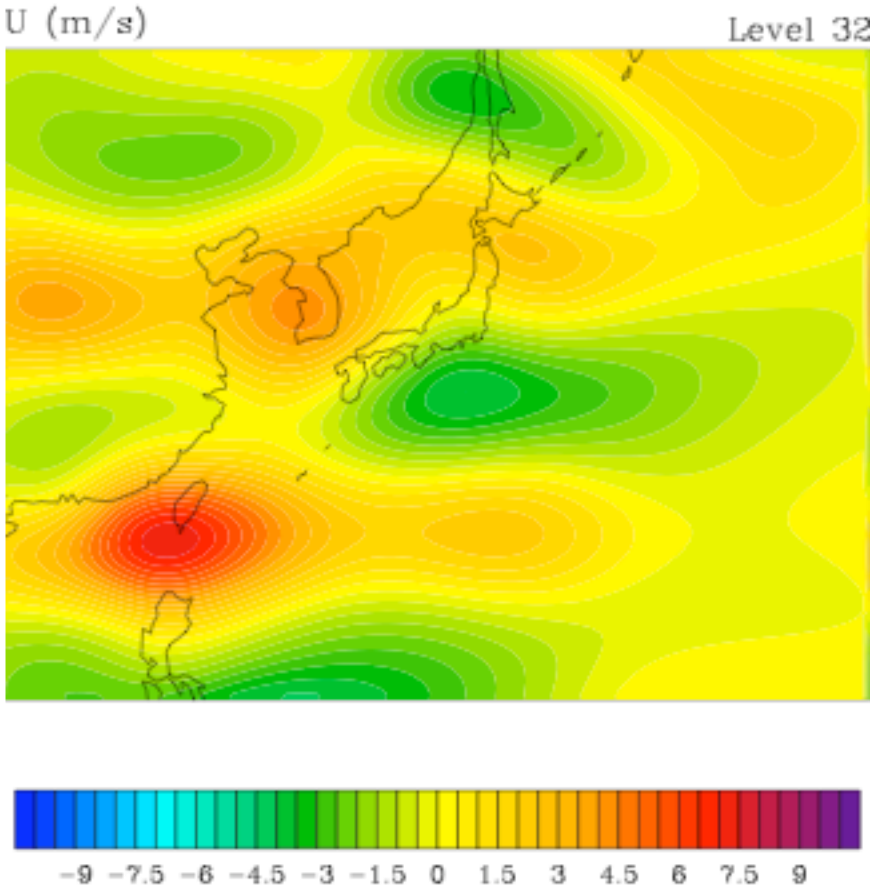
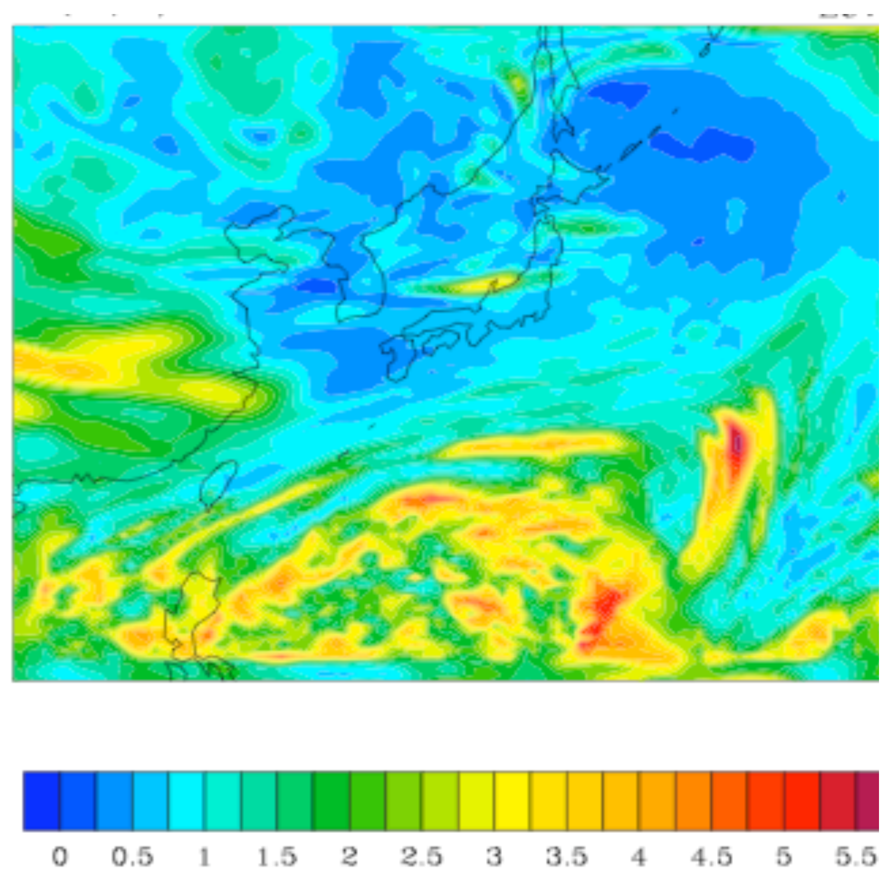
Ensemble Perturbations



WRF-Var Full Assimilation





U250 Analysis Increment

U250 Ensemble Spread

Control (no hybrid)

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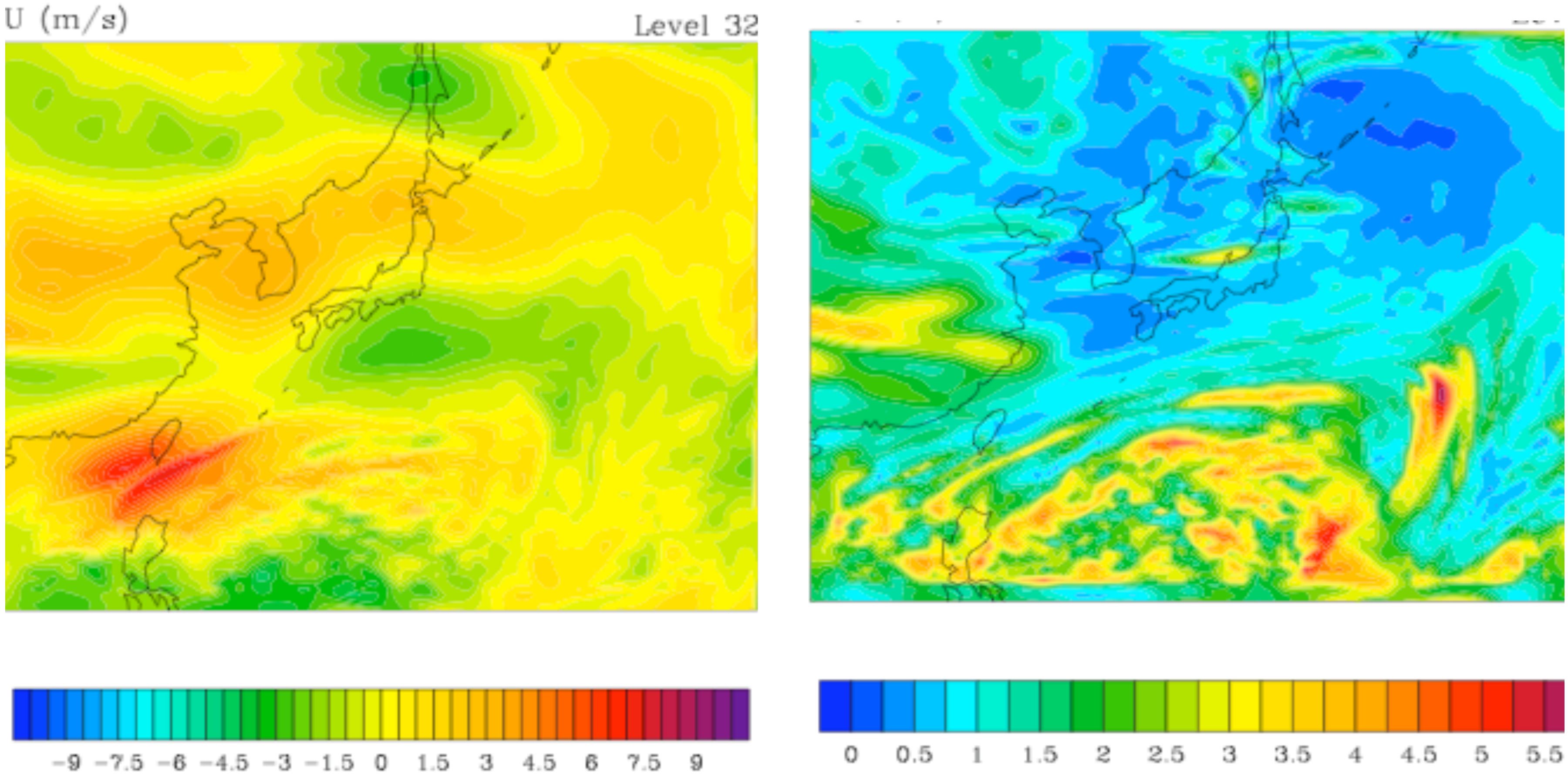
WRF-Var Full Assimilation



U250 Analysis Increment

U250 Ensemble Spread

W_e=2 , W_b=2

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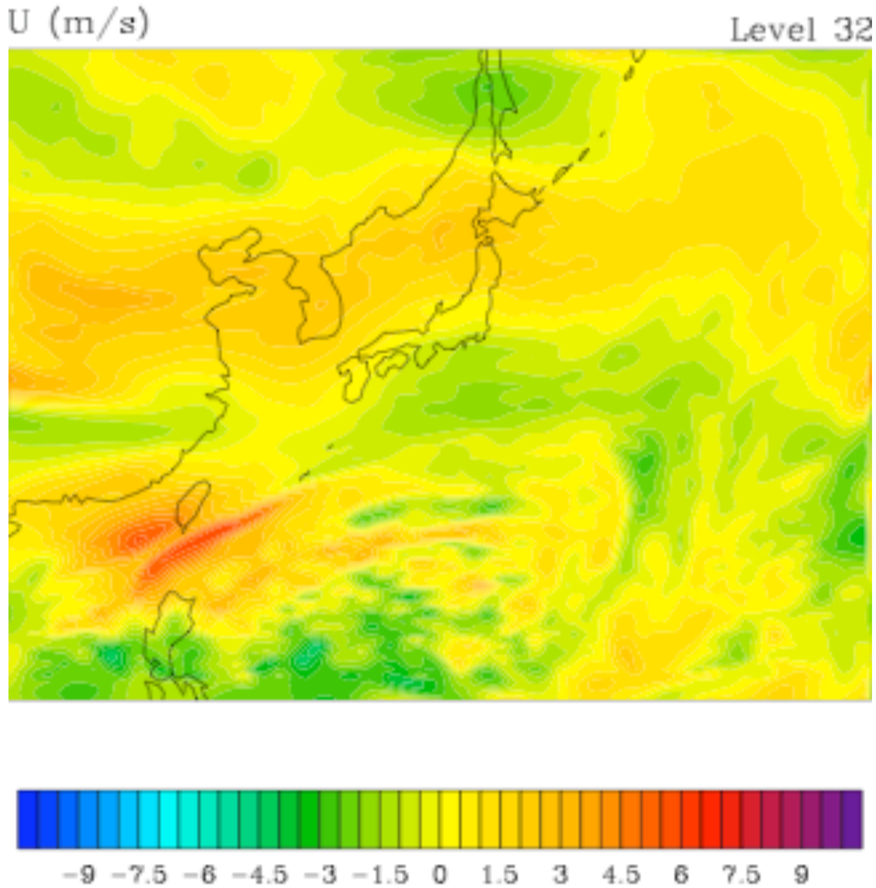
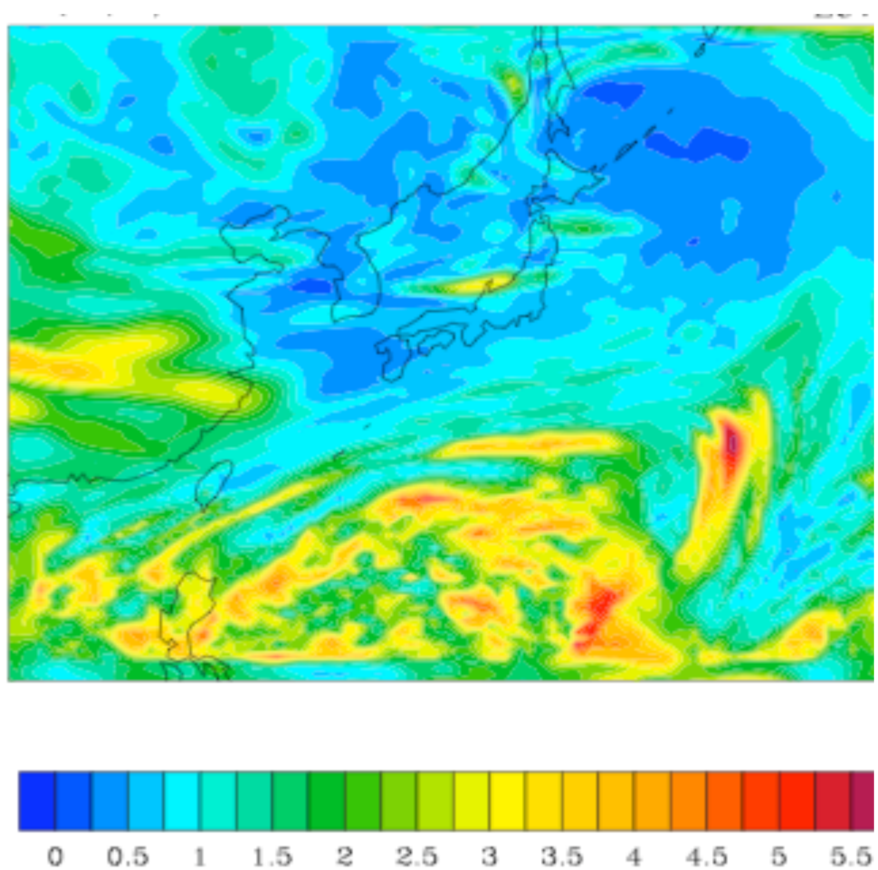
WRF-Var Full Assimilation



U250 Analysis Increment



U250 Ensemble Spread

W_e=1.25 , W_b=5

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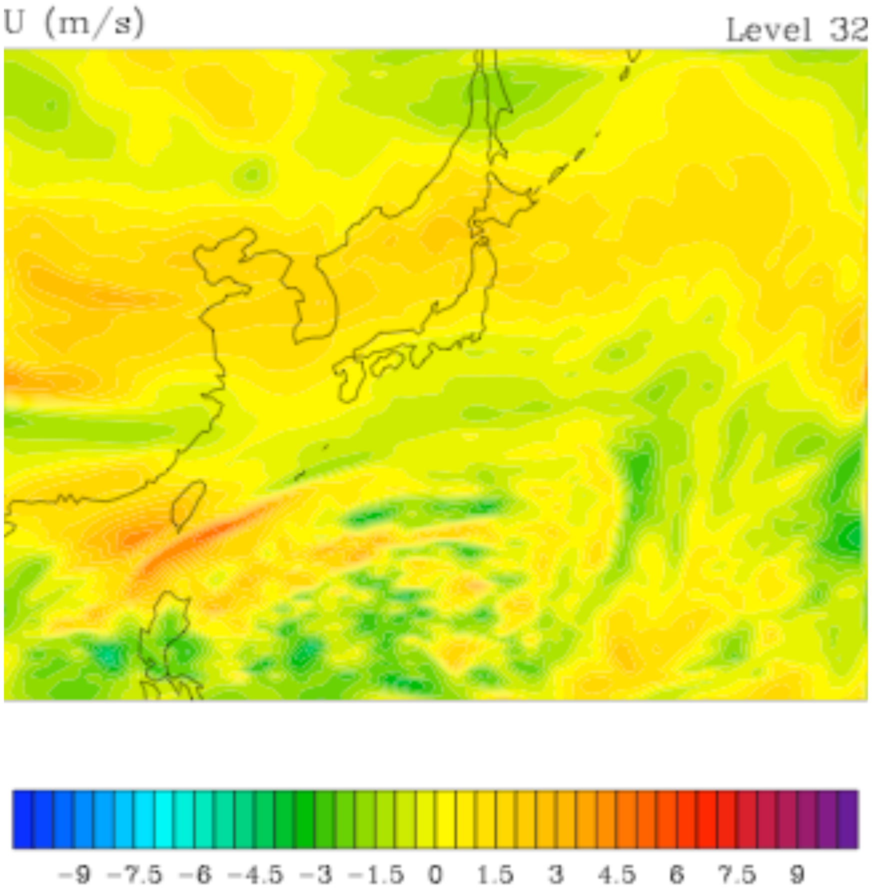
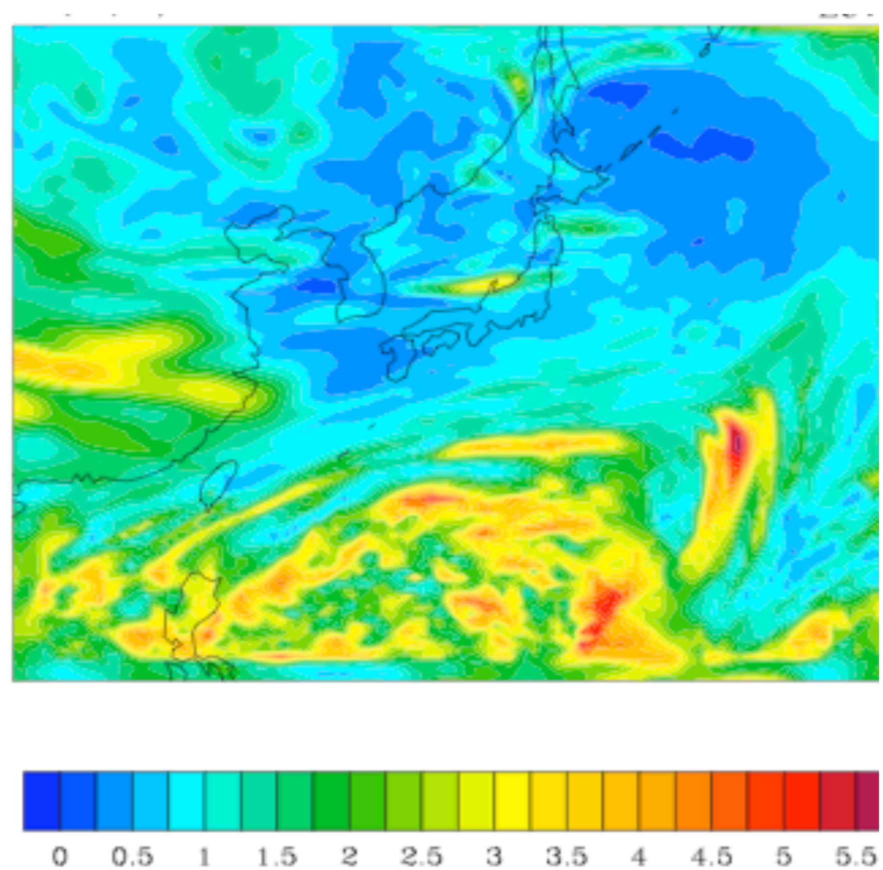
WRF-Var Full Assimilation



U250 Analysis Increment



U250 Ensemble Spread

W_e=1.1, W_b=11

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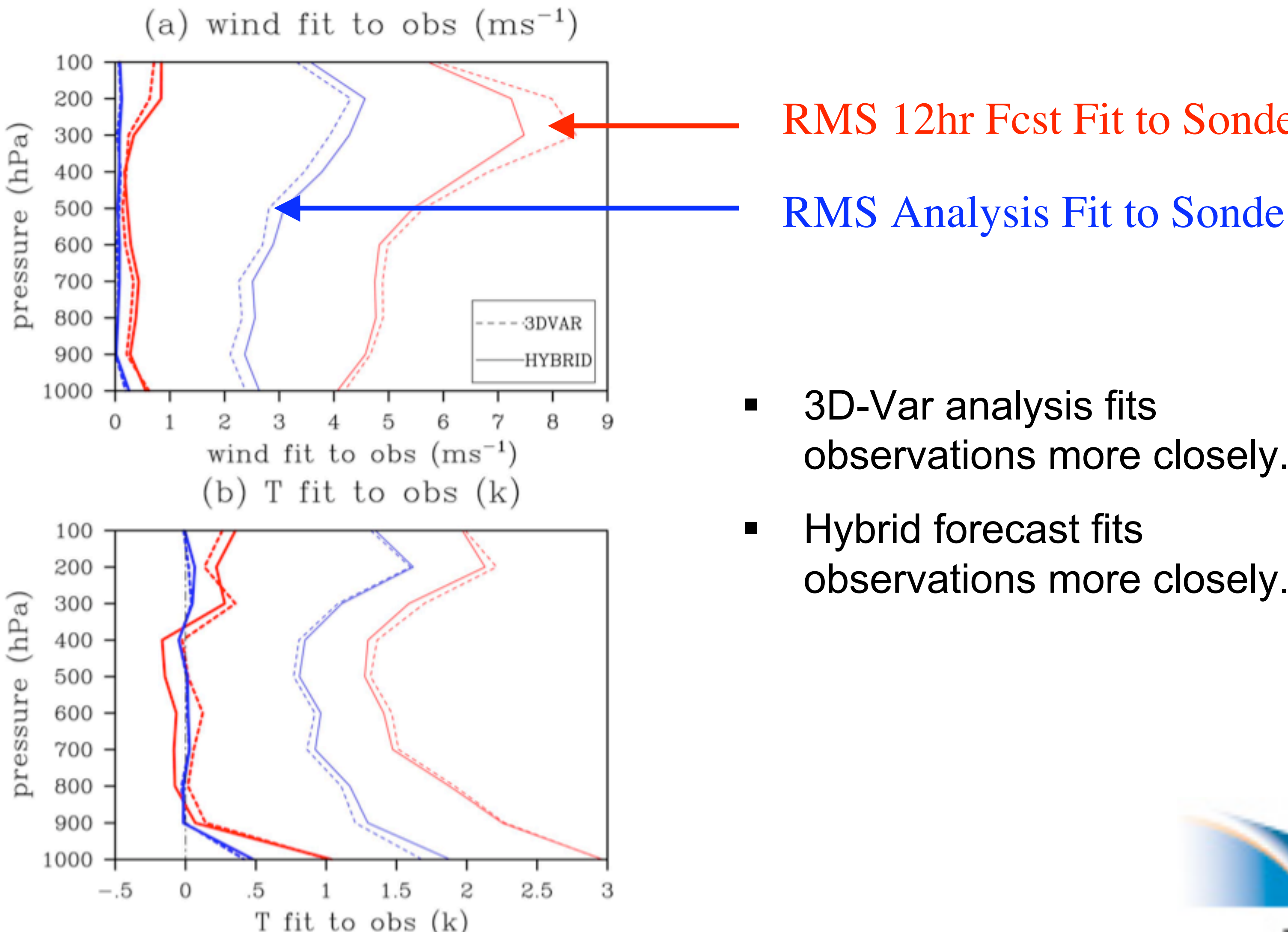
Hybrid 1-Month Real-Data (Sonde) Trial (Wang, Barker, Hamill and Snyder 2008b)



- 3D-Var analysis fits observations more closely.
- Hybrid forecast fits observations more closely.

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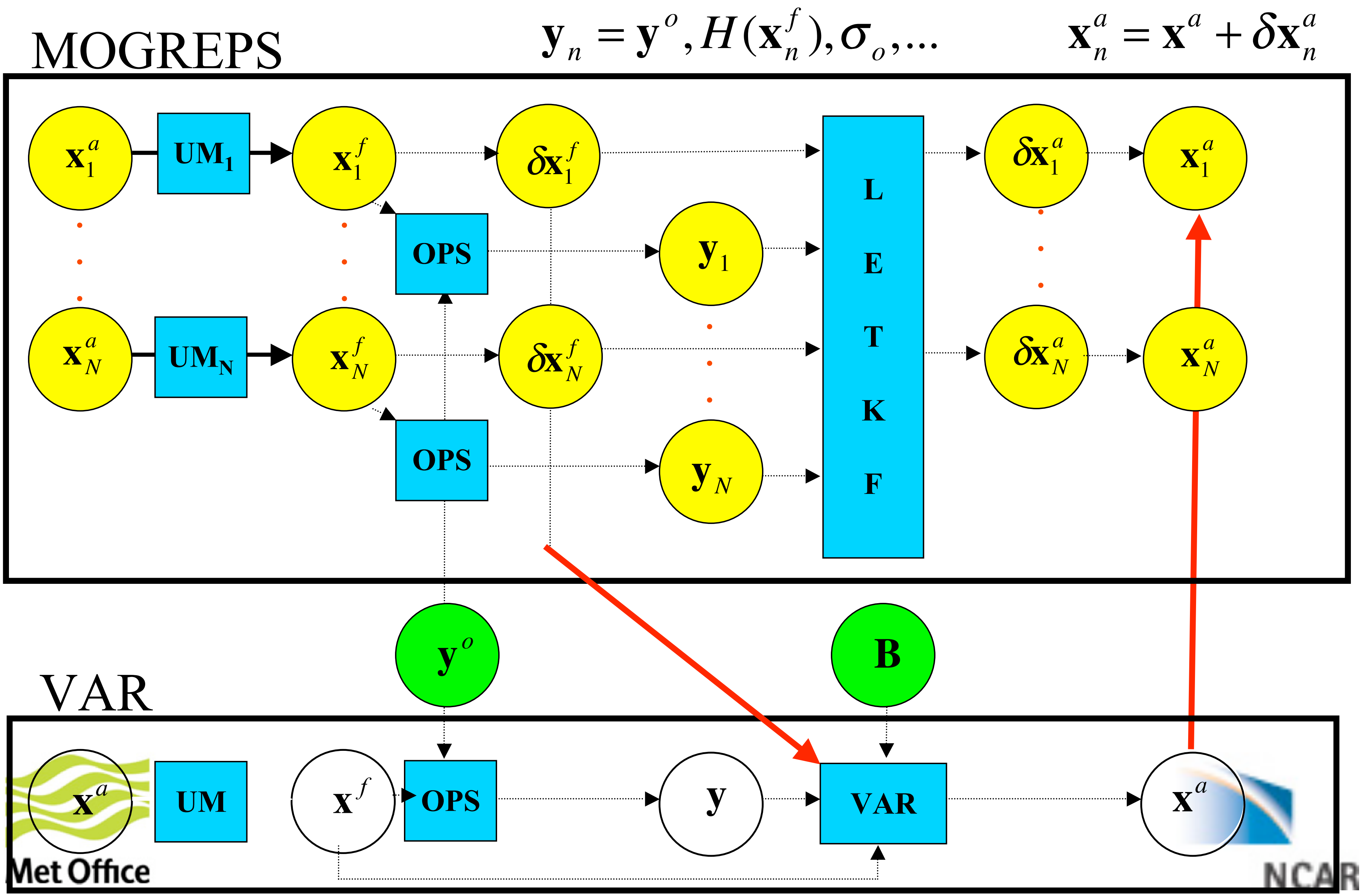
Met. Office 4D-Var/LETKF Hybrid System



Conclusions

- 4D-Var/EnKF solving same problem. Devil is in the detail.
- Distinction between variational/ensemble DA is blurred.
- Ensemble forecasting is here to stay. DA should make use of it.
- Hybrid in VAR shown. Hybrid in EF also possible.
- Flow-dependent covariances only one (now minor?) consideration. Bigger issues: non-Gaussianity, model error…..
- 'Seamless assimilation/prediction' implies flexible DA system.

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Questions

- Do we agree that the issue of flow-dependence in forecast error covariances is now a relatively 'solved' problem, and we should focus more on larger concerns e.g. non-Gaussianity, model error?

- Is the 4D-Var/EnKF computational cost comparison only an issue for those (fewer and fewer) centers running purely deterministic forecast systems?

- Will full operational implementations of EnKF really be 'simpler' than variational ones?

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