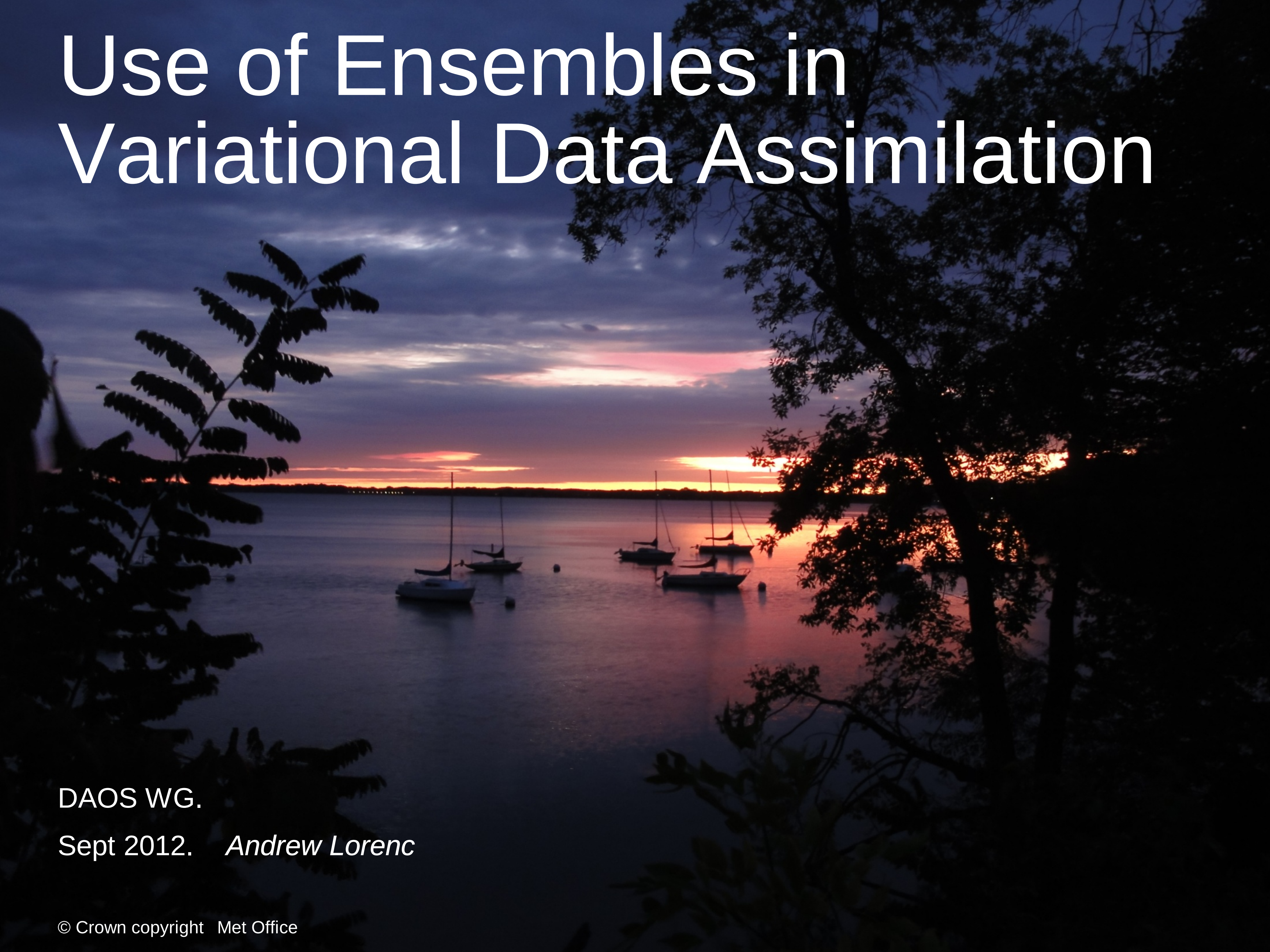
Use of Ensembles in Variational Data Assimilation



DAOS WG.

Sept 2012. *Andrew Lorenc*

1. Training climatological covariance models – assume ensemble perturbations are like background errors
2. Adding Errors Of The Day to Cov models – variances, scales etc.
3. Localised ensemble perturbations – the alpha control variable method
4. 4D covariances without using a linear model – 4DEnsemble-Var
5. Hybrid covariances – ways of compensating for a small ensemble.
6. How to generate the ensemble – a separate EnKF or an ensemble of VARs.
7. Some suggestions on terminology.

1. Training climatological covariance models

- Training from o-b (Hollingsworth & Lonnberg 1986) is less valid as ‘o’ errors increasingly dominate. Advanced methods using such statistics exist (Desroziers et al 2005)

- Train using model perturbation constructed to look like background errors:

  - Even the inventors disowned the NMC method (Parrish & Derber 1992)

  - Increasingly popular to **use ensemble perturbations as in the EnKF** (Fisher 2003)

  - However these do not properly sample model errors!

2. Adding Errors Of The Day to Cov models – variances, scales etc.

- ECMWF system (Slides from Massimo Bonavita via Carla who could not attend)

History

- CY37R2 (May 2011): Use of EDA Variances for ***balanced part*** of 4D-Var control vector and ***Quality Control*** of observations

- CY38R1 (June 2012): Re-calibration of ***JB*** based on more recent EDA + ***Revised Spectral Filter*** of EDA VARs

Main Research Developments

- Non-homogeneous Filtering of EDA Variances
- Extending the use of EDA Variances: Error Estimation for Unbalanced Control Vector
- On-line EDA Error Covariances.

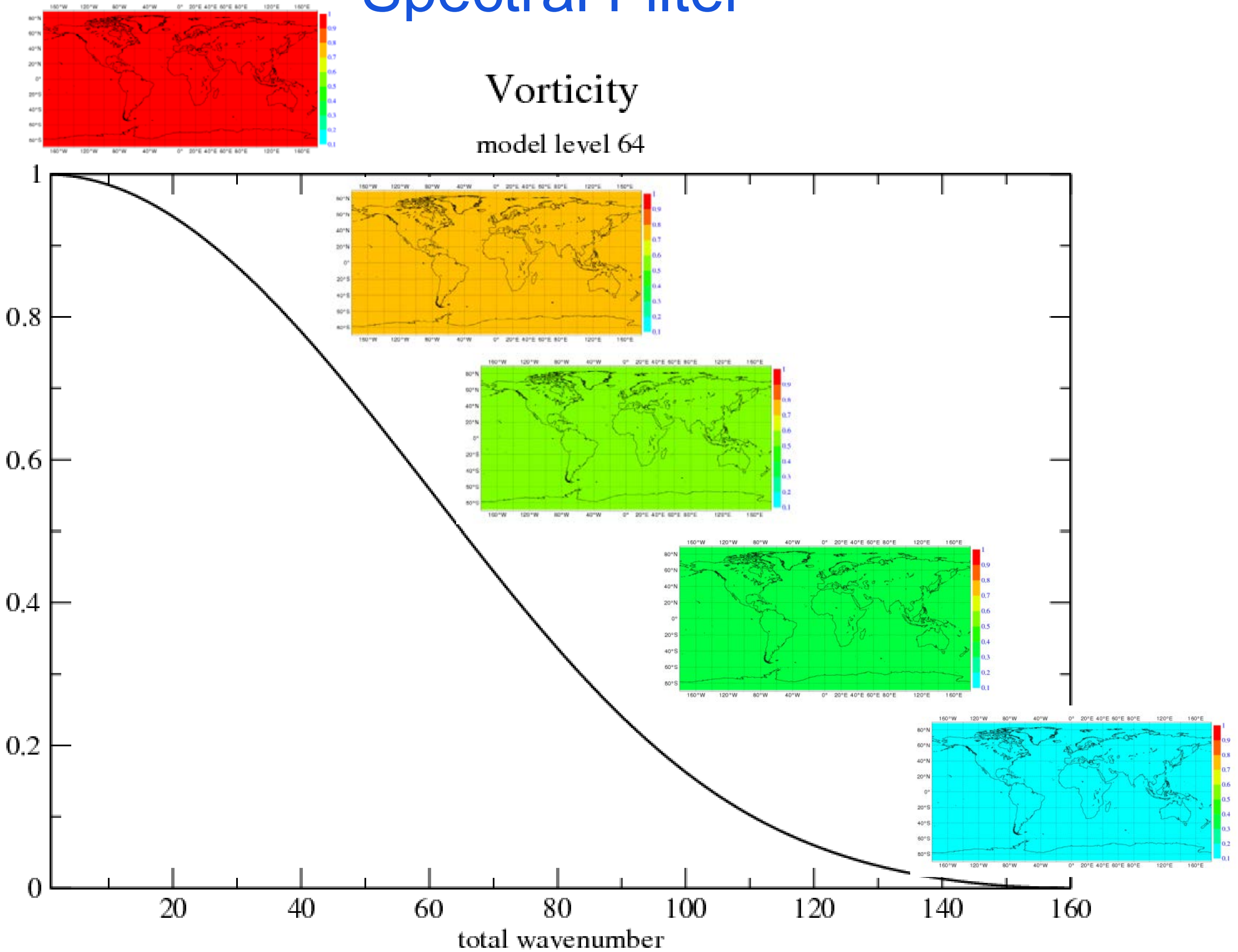
Non-homogeneous Filtering of EDA Variances

- Can we do anything better in terms of filtering?

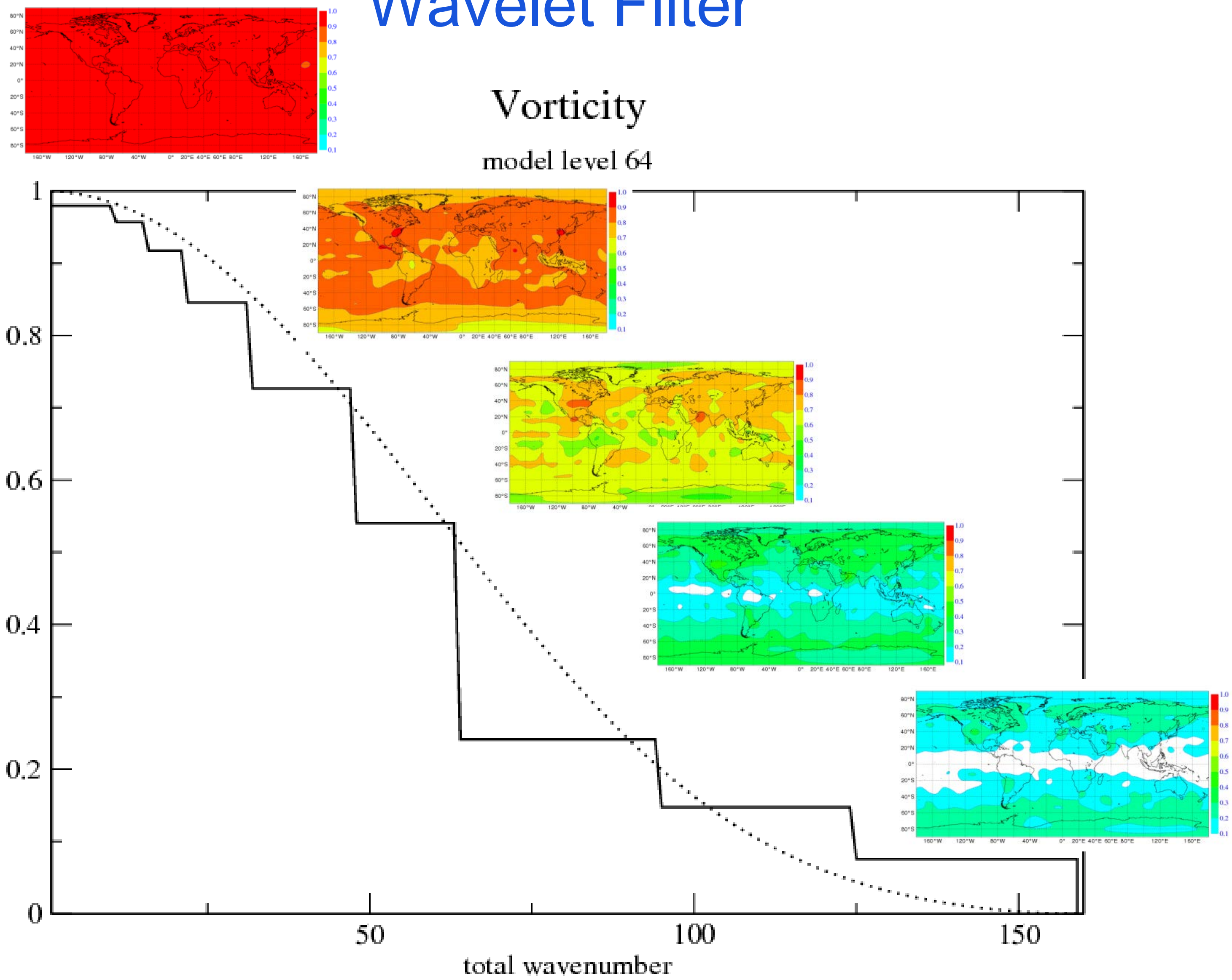
$$L_{noise} = L_{BG} / \sqrt{2}$$

- Since background error length scales are non-homogenous, noise filter should also be.
- Current spectral filter is spatially homogeneous.
- If a wavelet filter is instead used some geographical variability can be achieved

Spectral Filter

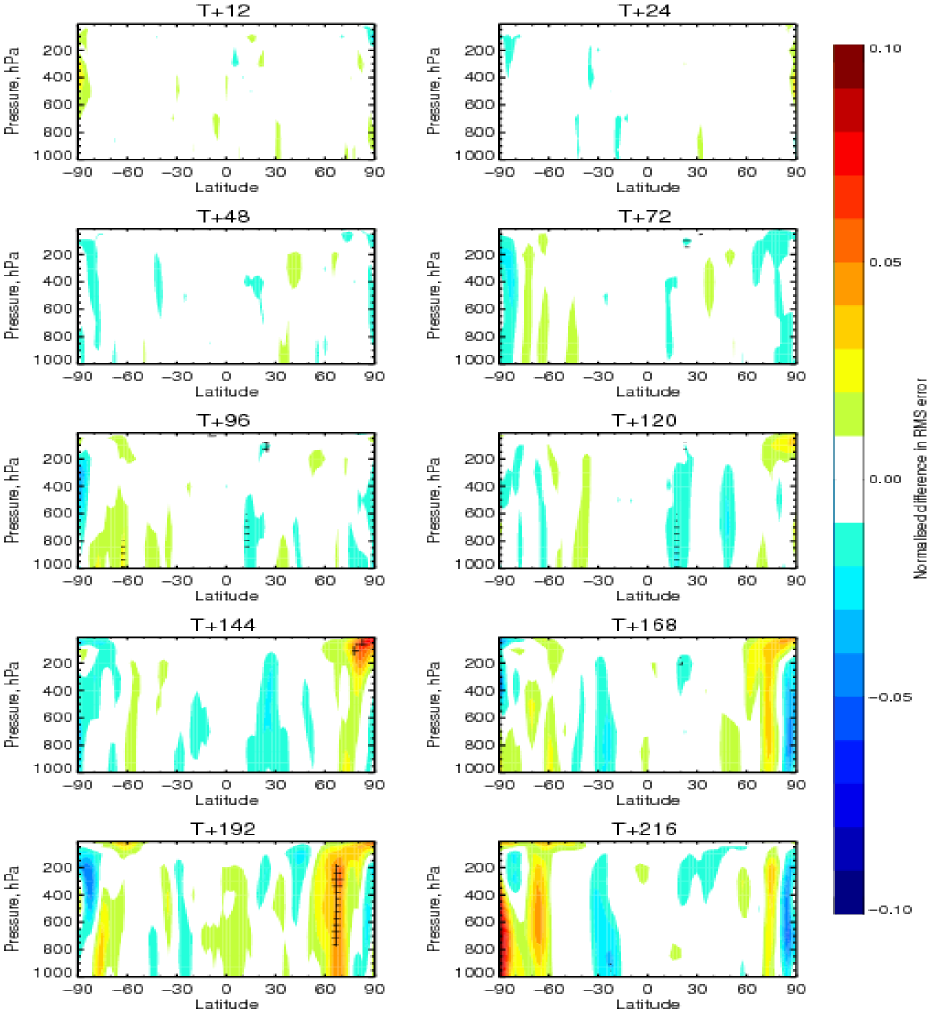


Wavelet Filter



Non-homogeneous Filtering of EDA Variances

- EDA 10 member
- **neutral** results on hybrid 4DVar
- will be tested with larger EDA



Z RMSE Wavelet Vorticity-Spectral
Verified against own analysis
Sep-Dec (+ 95% significant impact)

Extending the use of EDA Variances

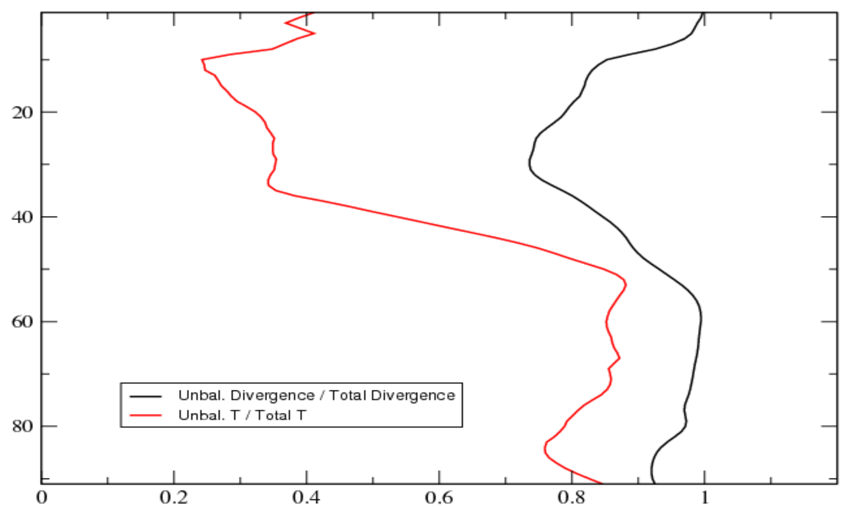
- EDA Variances for the **Unbalanced Control Vector** (η_u, $(T,p_s)_u$).

$$\zeta = \zeta$$
$$\eta = \mathbf{M}\zeta + \eta_u$$
$$(T, p_s) = \mathbf{N}\zeta + \mathbf{P}\eta_u + (T, p_s)_u$$

$\Rightarrow$

$$Var(\zeta) = Var(\zeta)$$
$$Var(\eta) = \mathbf{M}Var(\zeta)\mathbf{M}^T + Var(\eta_u)$$
$$Var(T, p_s) = \mathbf{N}Var(\zeta)\mathbf{N}^T + \mathbf{P}Var(\eta_u)\mathbf{P}^T + Var(T, p_s)_u$$

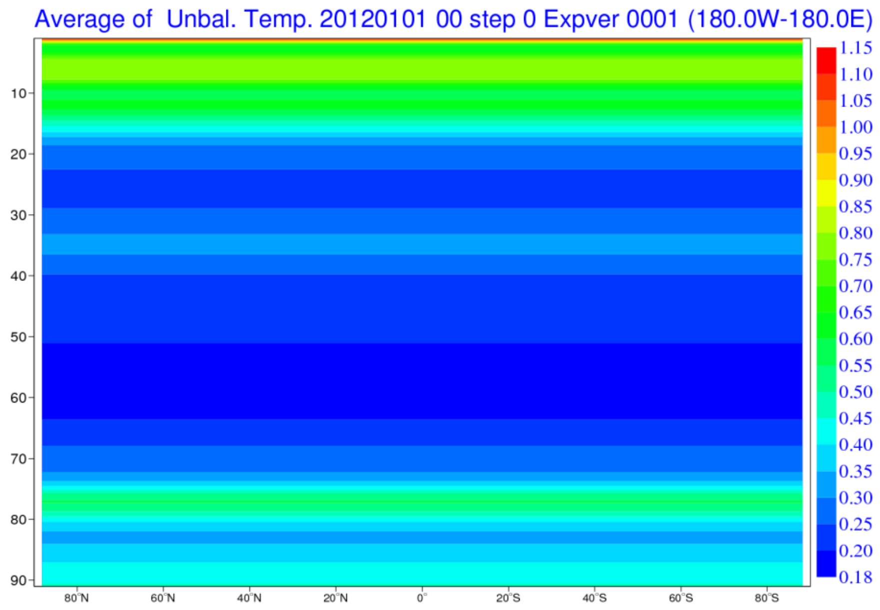
Unbalanced / Total Error Variances



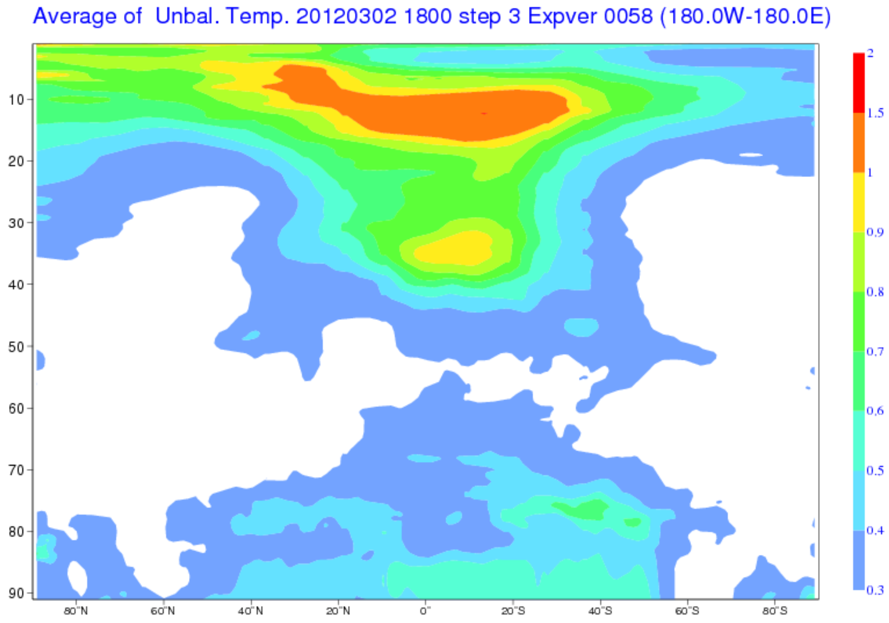
Extending the use of EDA Variances

EDA Variances for **Unbalance Control Vector**

Current BG error variance for Unbal. Temp.



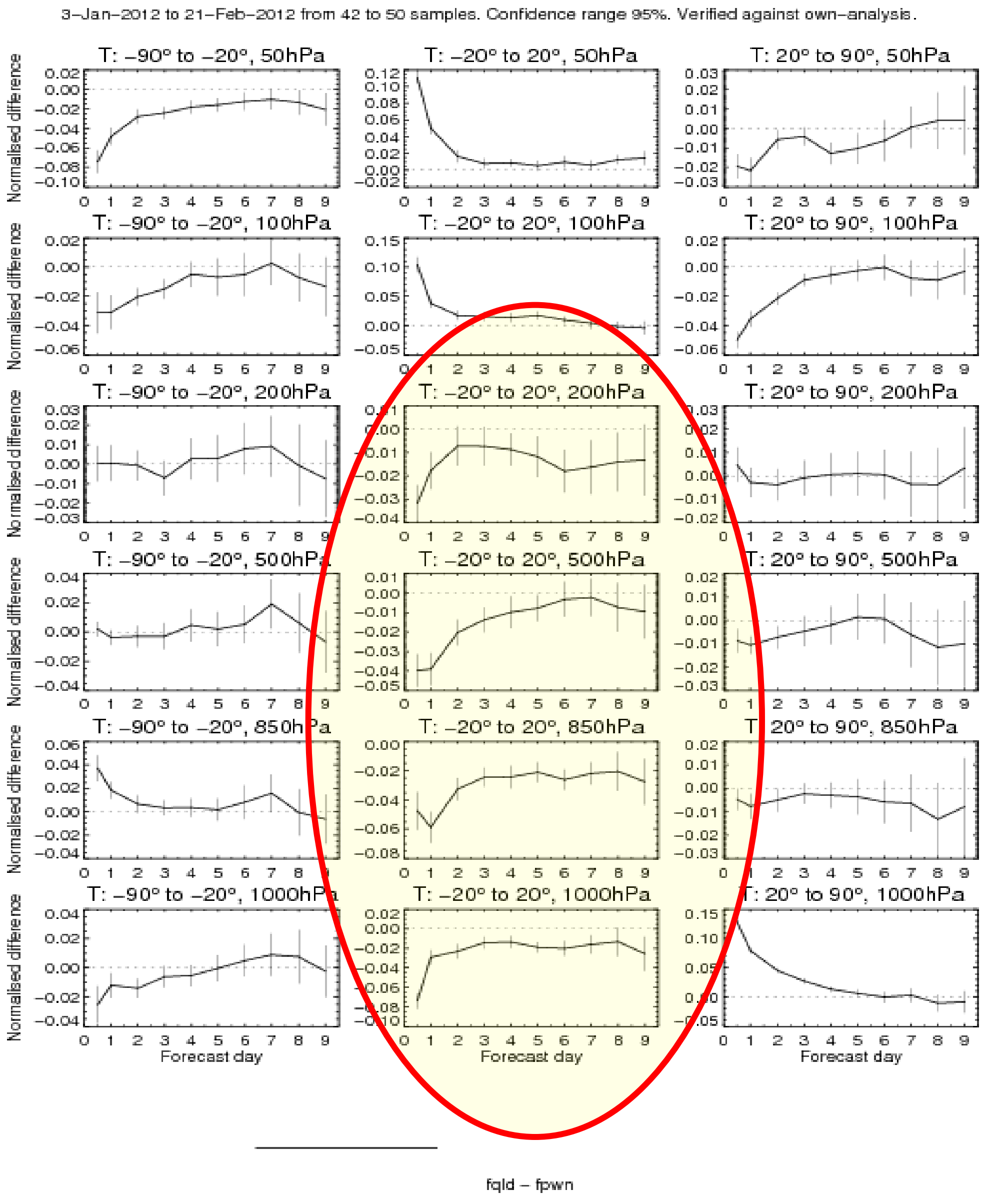
EDA BG Error variance for Unbal. Temp.



ECMWF

Extending the use of EDA Variances

38R1 T511L91
Temperature
RMSE reduction



ECMWF

EDA Covariances

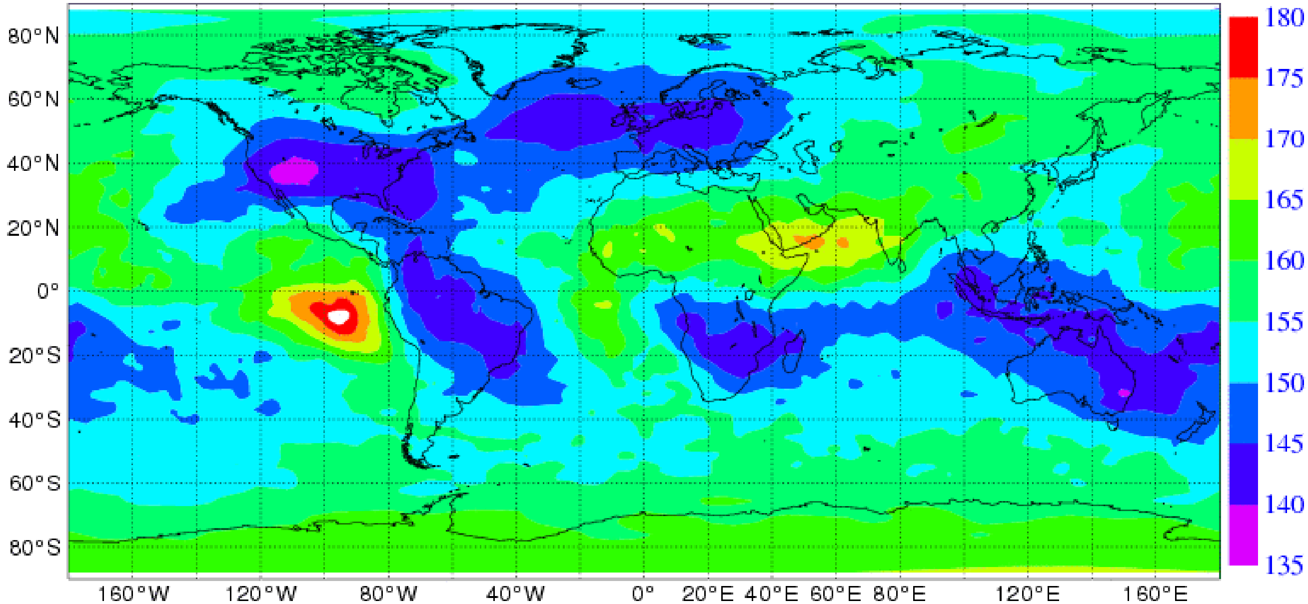
$$\left(\mathbf{x}-\mathbf{x}_b\right)=\mathbf{T}^{-1}\mathbf{\Sigma}_b^{1/2}\sum_j \psi_j \otimes\left[\mathbf{C}_j^{1/2}(\lambda,\phi)\chi_j\right]$$

$\mathbf{C}_j(\lambda,\varphi)$ are full vertical covariance matrices, function of (λ,φ). They determine both the horizontal and vertical background error *correlation structures* => "*wavelet JB*"

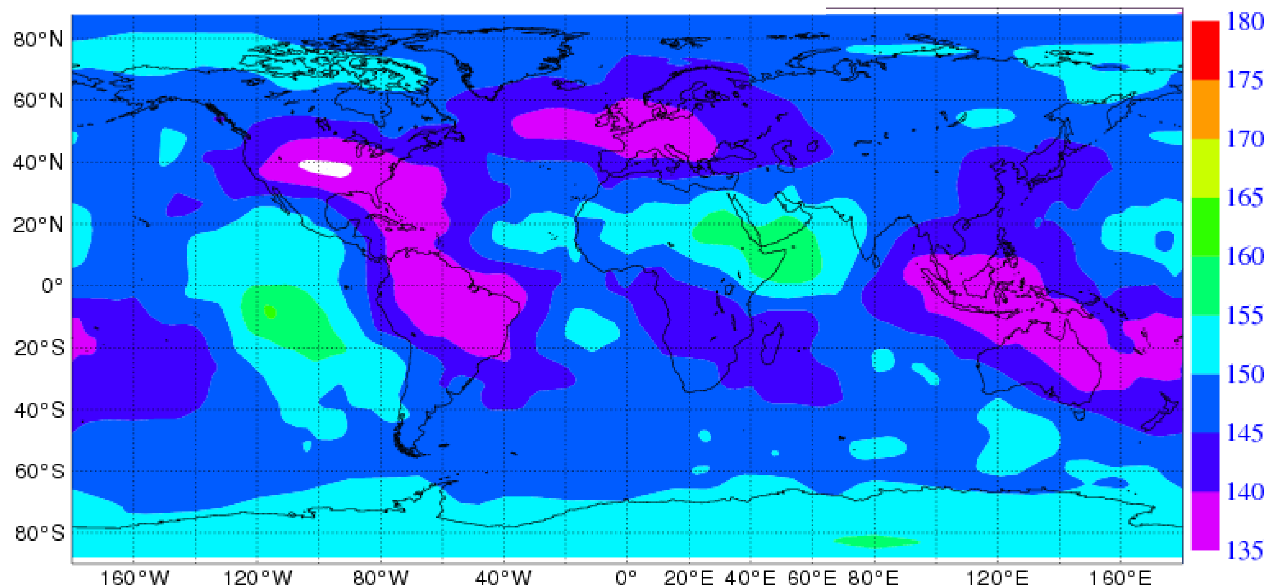
flow-dependent EDA estimates of $\mathbf{\Sigma}_b$ and $\mathbf{C}_j(\lambda,\varphi)$

To compensate the small EDA sample size → EDA past 30 days are considered

Correlation Length Scale of Vorticity errors, ~200 hPa



Online wavelet JB, 30 days running avg Feb.-May 2012



Operational Static wavelet JB

Massimo Bonavita

EDA Covariances

- Error covariance length scales are mainly sensitive to:

  A. Observation distribution and density;

  B. Flow characteristics (i.e. spatial distribution of weather systems)

- 30 days running average JB captures changes in A. (very relevant for Re-analysis applications) and intra-seasonal variations of B.

- Larger EDA would allow a larger fraction of "errors of the day" to be represented

3. Localised ensemble perturbations – the alpha control variable method

- Met Office code written in late 90's for 3D-Var or 4D-Var (Barker and Lorenc) then shelved pending an ensemble.
- Proven to work in NCAR 3D-Var (Wang et al. 2008)
- Proven to be equivalent to EnKF localisation (Lorenc 2003, Wang et al 2007).
- Eventually implemented in Met Office operational global hybrid ensemble-4D-Var (Clayton et al 2012).
- Widely used.

En-Var formulation: Preconditioning

- Preconditioned cost function formulation at Environment Canada:

$$\boxed{J(\xi)=\frac{1}{2}(H_{4D}[\mathbf{x}_b]+\mathbf{H}\Delta\mathbf{x}(\xi)-\mathbf{y})^T\mathbf{R}^{-1}(H_{4D}[\mathbf{x}_b]+\mathbf{H}\Delta\mathbf{x}(\xi)-\mathbf{y})+\frac{1}{2}\xi^T\xi}$$

- In En-Var with hybrid covariances, the control vector (ξ) is made up of 2 vectors:

$$[\xi]=\begin{bmatrix}\xi_{\text{nmc}}\\ \xi_{\text{ens}}\end{bmatrix} \rightarrow \quad [\xi_{\text{ens}}]=\begin{bmatrix}\xi_{\text{ens}}^{1}\\ \vdots\\ \xi_{\text{ens}}^{N_{\text{ens}}}\end{bmatrix}$$

- The analysis increment is computed as:

$$\boxed{\Delta\mathbf{x}(\xi)=\beta_{\text{nmc}}\mathbf{B}_{\text{nmc}}^{1/2}\xi_{\text{nmc}}+\beta_{\text{ens}}\sum_{k=1}^{N_{\text{ens}}}\mathbf{e}_k\circ\left(\mathbf{L}^{1/2}\xi_{\text{ens}}^{k}\right)}$$

- Appears to be better preconditioned than original “alpha control vector” formulation (in which $\mathbf{L}^{-1}$ and $1/\beta$ are in background term of J), especially when one of the β weights is small

- Appears some studies have used original “alpha control vector” formulation → what is impact? need for clarification in literature?

Hybrid VAR formulation

- VAR with climatological covariance $\mathbf{B}_c$:

$$\mathbf{B}_\mathbf{c} = \mathbf{U}\mathbf{U}^\mathrm{T} \qquad\qquad \delta\boldsymbol{x}_c = \mathbf{U}\boldsymbol{v} = \mathbf{U}_\mathrm{p}\mathbf{U}_\mathrm{v}\mathbf{U}_\mathrm{h}\boldsymbol{v}$$

- VAR with localised ensemble covariance $\mathbf{P}_e \circ \mathbf{C}_{loc}$:

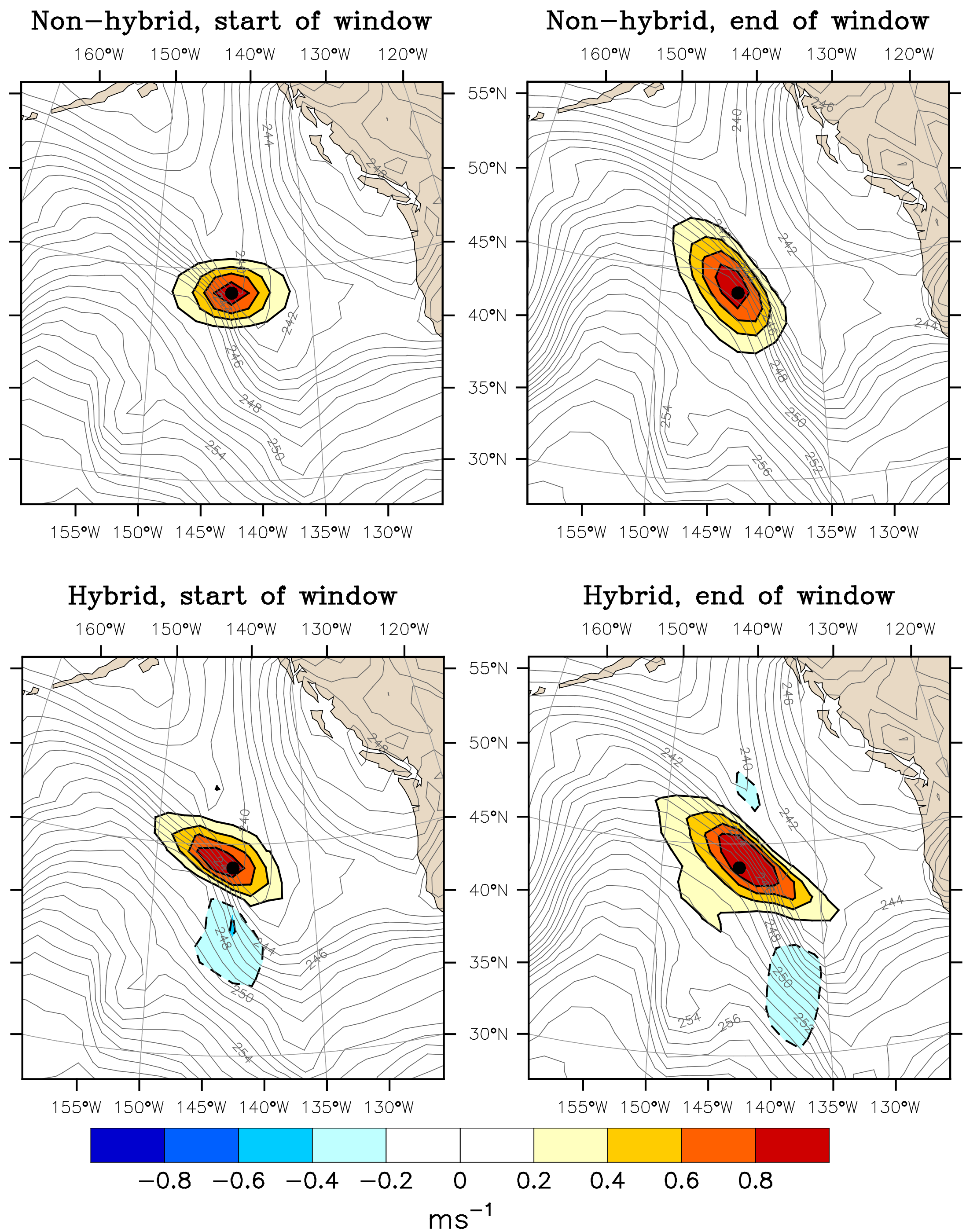
$$\mathbf{C}_{loc} = \mathbf{U}^\alpha \mathbf{U}^{\alpha\mathrm{T}} \qquad \boldsymbol{\alpha}_i = \mathbf{U}^\alpha \boldsymbol{v}_i^\alpha \qquad \delta\boldsymbol{x}_e = \frac{1}{\sqrt{K-1}} \sum_{i=1}^{K} (\boldsymbol{x}_i\text{-}\overline{\boldsymbol{x}}) \circ \boldsymbol{\alpha}_i$$

- **Note**: We are now modelling $\mathbf{C}_{loc}$ rather than the full covariance $\mathbf{B}_c$.
- Hybrid VAR:

$$\delta\mathbf{x} = \underline{\beta_c}\delta\mathbf{x}_c + \underline{\beta_e\delta\mathbf{x}_e} \qquad J = \frac{1}{2}\boldsymbol{v}^T\boldsymbol{v} + \underline{\frac{1}{2}\boldsymbol{v}^{\alpha T}\boldsymbol{v}^\alpha} + J_o + J_c$$

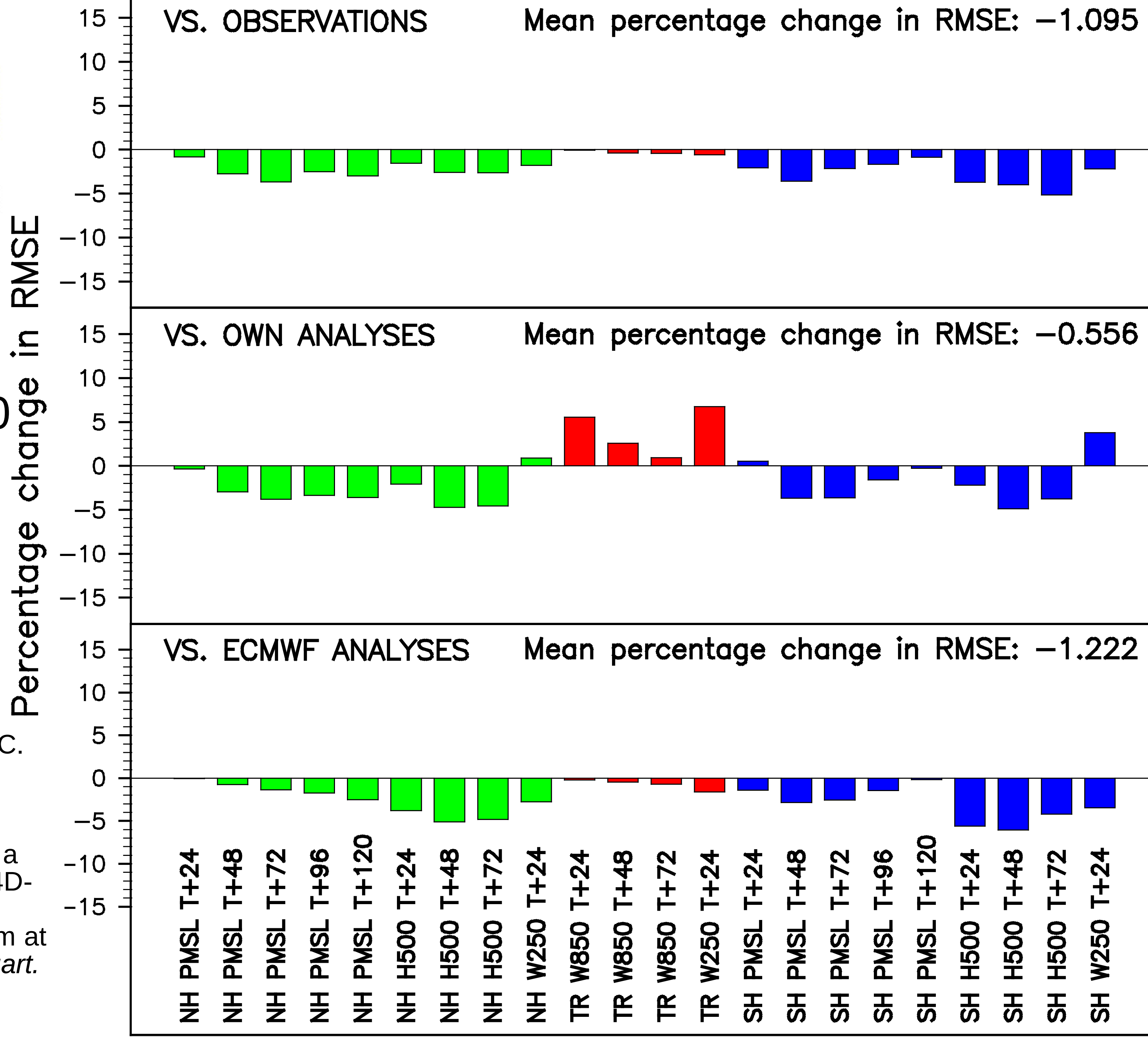
- **Met Office detail**: We localise and combine in transformed variable space to preserve balance and allow a nonlinear $\mathbf{U}_\mathrm{p}$.

Clayton, A. M., A. C. Lorenc and D. M. Barker 2012: Operational implementation of a hybrid ensemble/4D-Var global data assimilation system at the Met Office. *Quart. J. R. Met. Soc.*, **to appear**



Zonal wind responses (filled thick contours, with negative contours dashed) to a single zonal wind observation at the start (left-hand plots) and end (right-hand plots) of the 6-hour 4D-Var window. The plots are for the same time and model level (\approx500 hPa) as the observation. Upper plots are for the non-hybrid configuration; lower plots for the hybrid configuration used within the pre-operational trials. The observation location is marked with a black dot at the centre of each plot. The unfilled contours show the background temperature field.

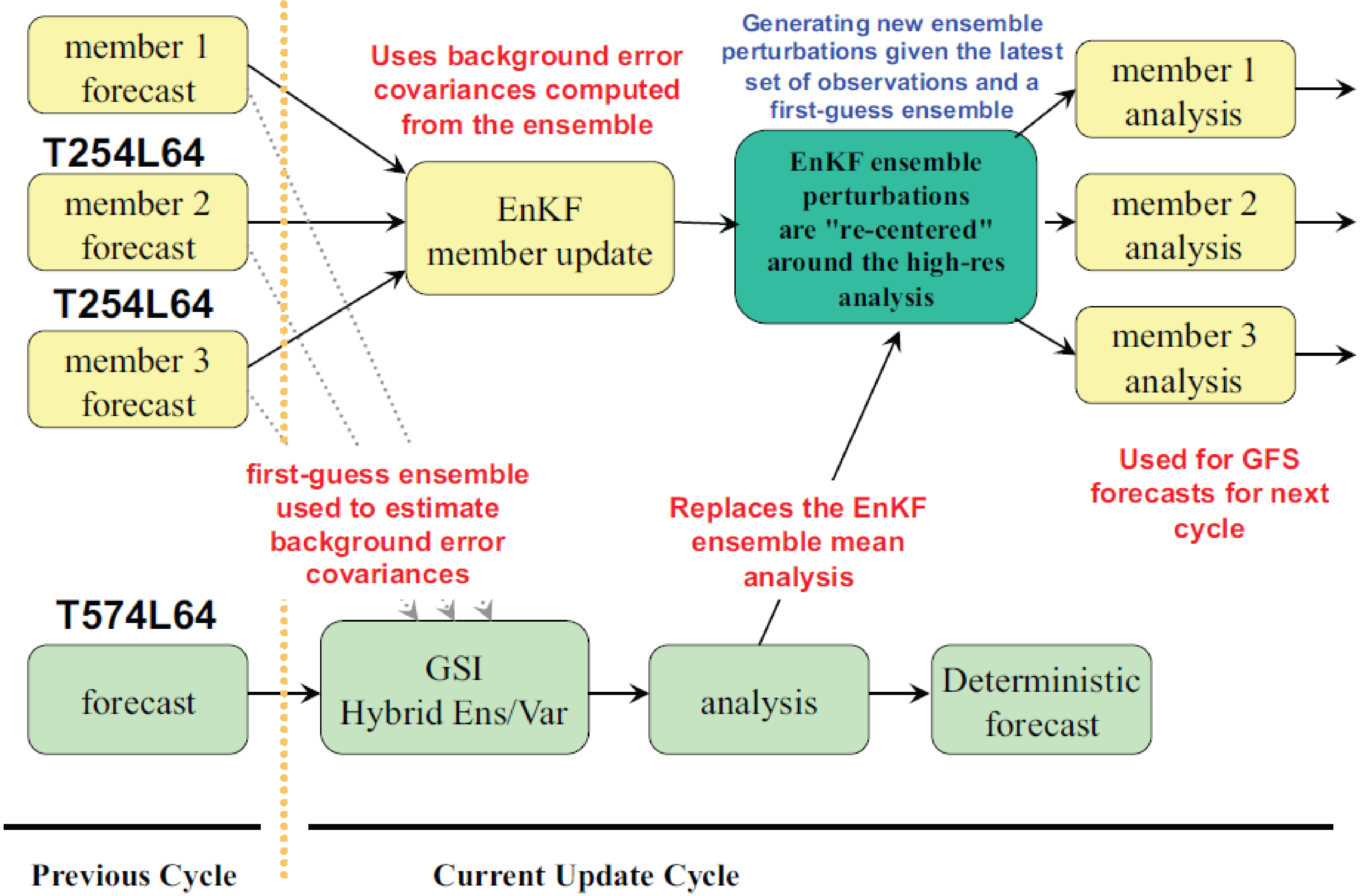
Results from June 2010 parallel trial



Clayton, A. M., A. C. Lorenc and D. M. Barker 2012: Operational implementation of a hybrid ensemble/4D-Var global data assimilation system at the Met Office. *Quart. J. R. Met. Soc.*, **to appear**

NCEP GDAS upgrade 22 May 2012

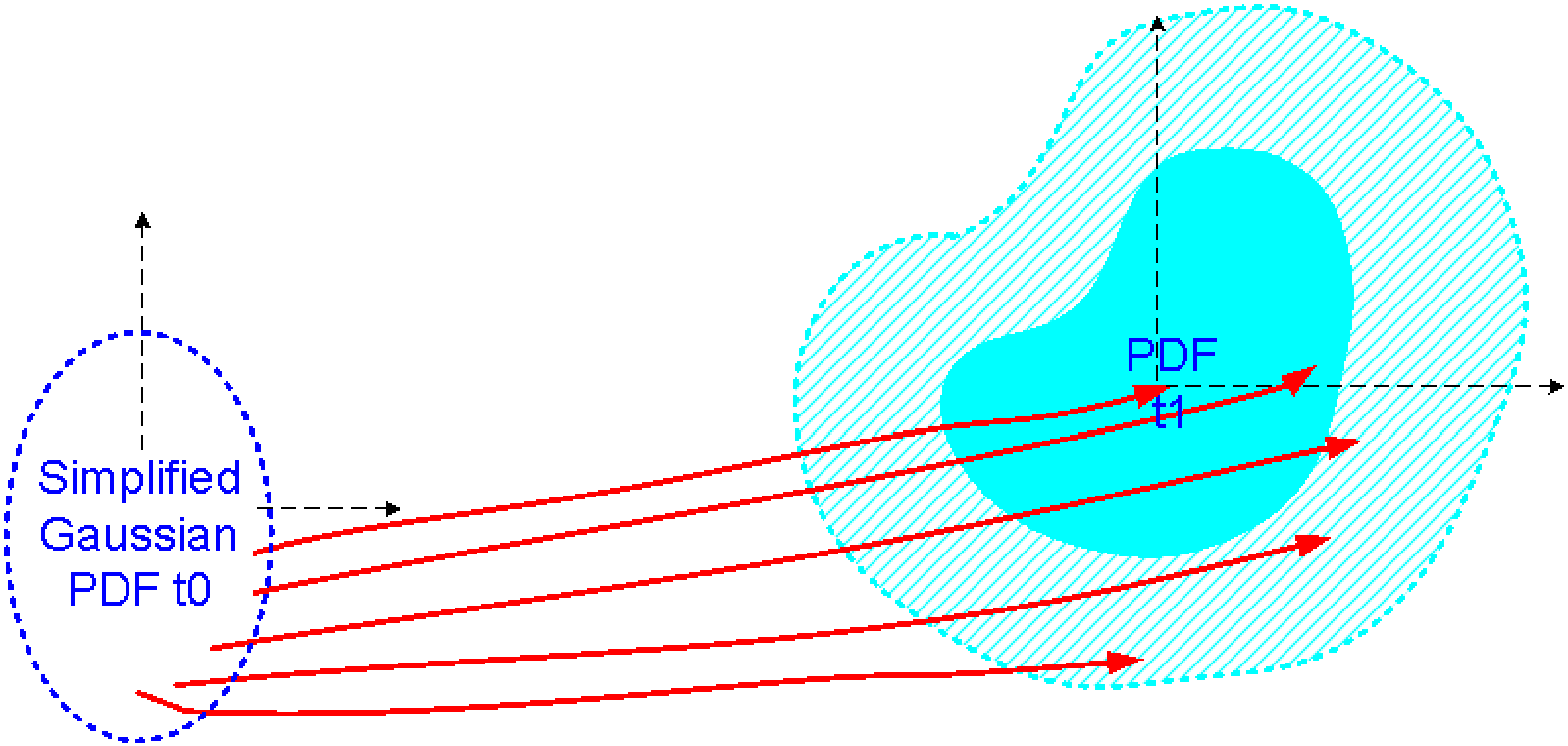
Dual-Resolution Coupled Hybrid 3D-VAR/EnKF



4. 4D covariances without using a linear model – 4DEnsemble-Var

- Combination of ideas from alpha-CV just discussed and 4DEnKF (Hunt et al 2004).
- First published by Liu et al (2008) and tested for real system by Buehner et al (2010).
- Potentially equivalent to 4D-Var without needing linear and adjoint model software.
- Model forecasts can be done in parallel beforehand rather than sequentially during the 4D-Var iterations.
- Toy model comparisons (Andrew)
- Canadian expts with aim of replacing 4D-Var in 2013 (Mark)
- Met Office system enabling an ensemble of 4D-En-Var.

Deterministic 4D-Var

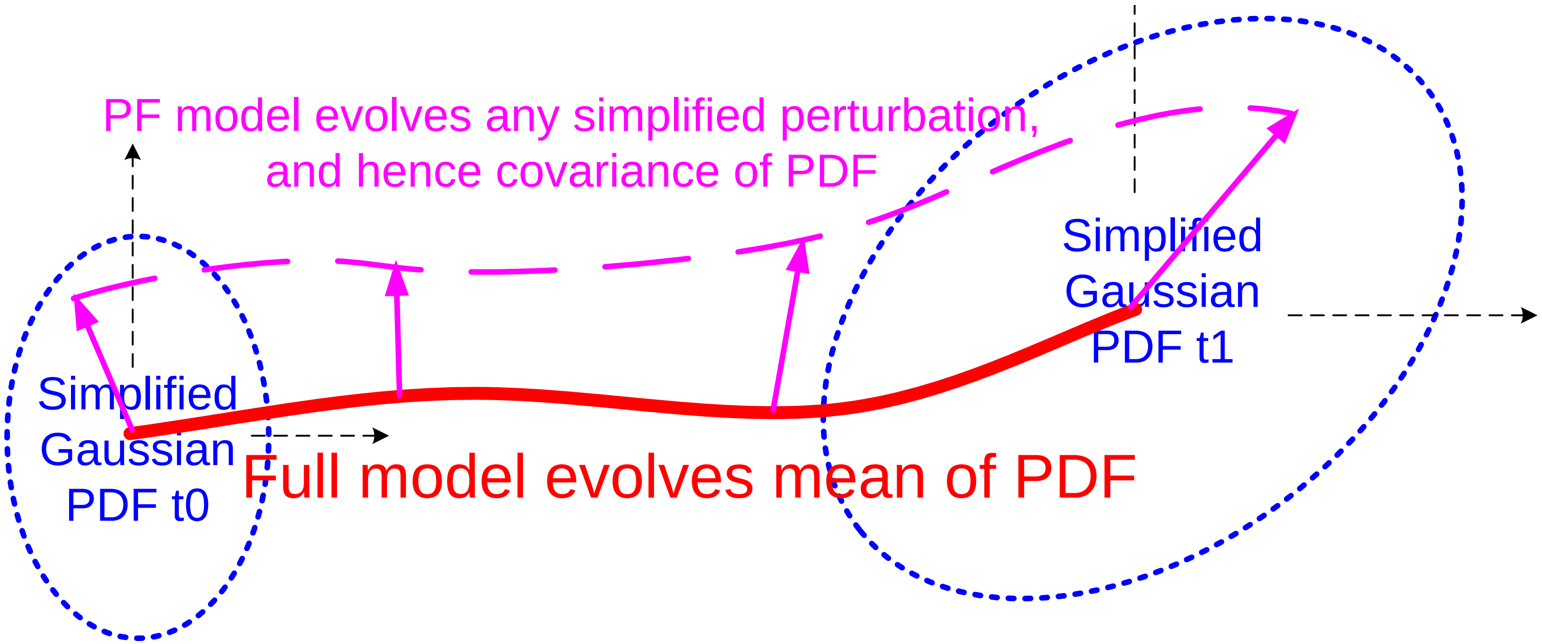


Initial PDF is approximated by a Gaussian.

Descent algorithm only explores a small part of the PDF, on the way to a local minimum.

4D analysis is a trajectory of the full model,

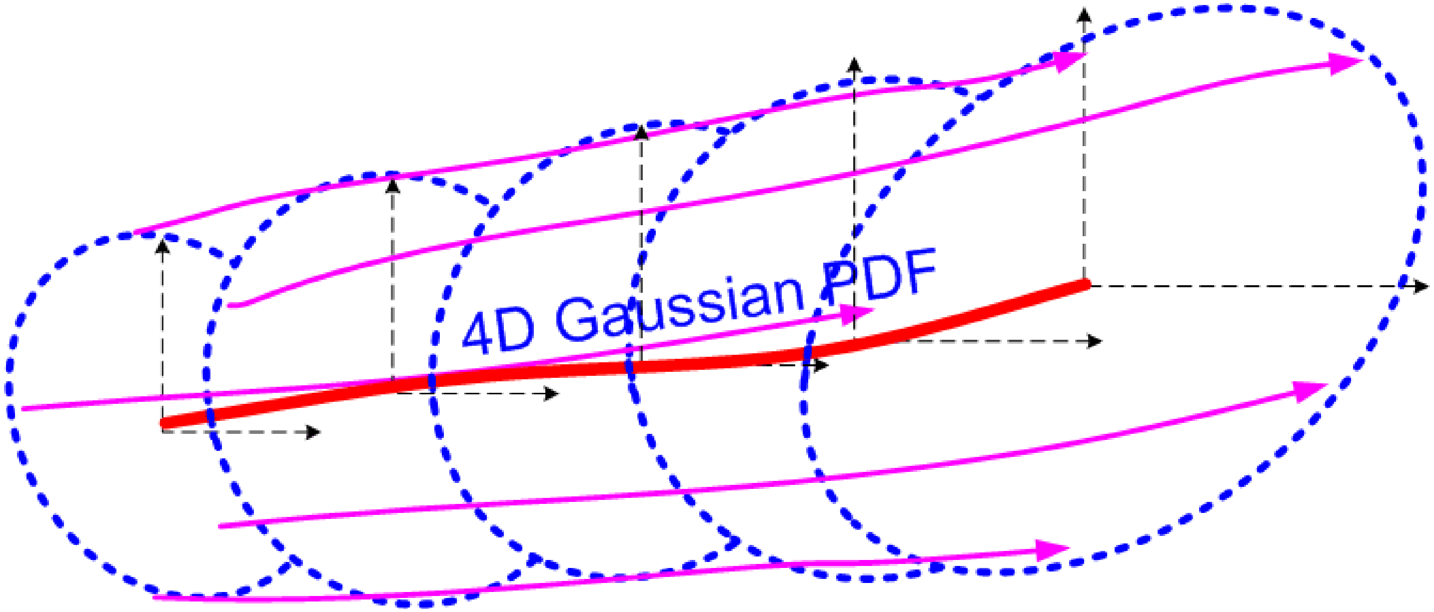
Statistical, incremental 4D-Var



Statistical 4D-Var approximates entire PDF by a Gaussian.

4D analysis increment is a trajectory of the PF model,

Incremental 4D-Ensemble-Var



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.

En-Var formulation

- In 4D-Var the 3D analysis increment is evolved in time using the TL/AD forecast model (here included in $\mathbf{H}_{4D}$):

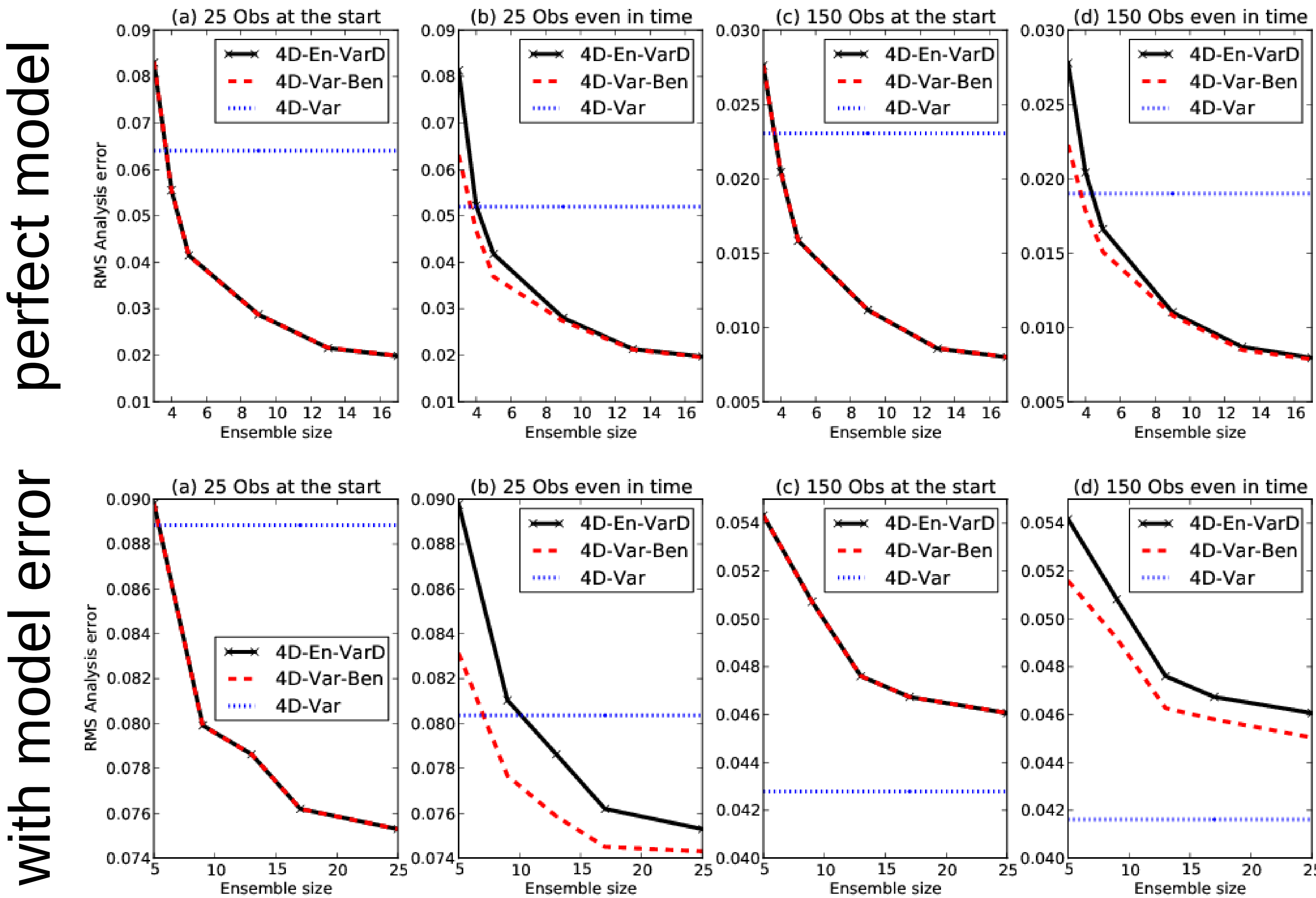
$$J(\Delta\mathbf{x}) = \frac{1}{2}(H_{4D}[\mathbf{x}_b] + \mathbf{H}_{4D}\Delta\mathbf{x} - \mathbf{y})^T \mathbf{R}^{-1}(H_{4D}[\mathbf{x}_b] + \mathbf{H}_{4D}\Delta\mathbf{x} - \mathbf{y}) + \frac{1}{2}\Delta\mathbf{x}^T \mathbf{B}^{-1}\Delta\mathbf{x}$$

- In En-Var the background-error covariances and analysed state are explicitly 4-dimensional, resulting in cost function:

$$J(\Delta\mathbf{x}_{4D}) = \frac{1}{2}(H_{4D}[\mathbf{x}_b] + \mathbf{H}\Delta\mathbf{x}_{4D} - \mathbf{y})^T \mathbf{R}^{-1}(H_{4D}[\mathbf{x}_b] + \mathbf{H}\Delta\mathbf{x}_{4D} - \mathbf{y}) + \frac{1}{2}\Delta\mathbf{x}_{4D}{}^T \mathbf{B}_{4D}^{-1}\Delta\mathbf{x}_{4D}$$

- Computations involving ensemble-based $\mathbf{B}_{4D}$ can be more expensive than with $\mathbf{B}_{nmc}$ depending on ensemble size and spatial resolution, but significant parallelization is possible

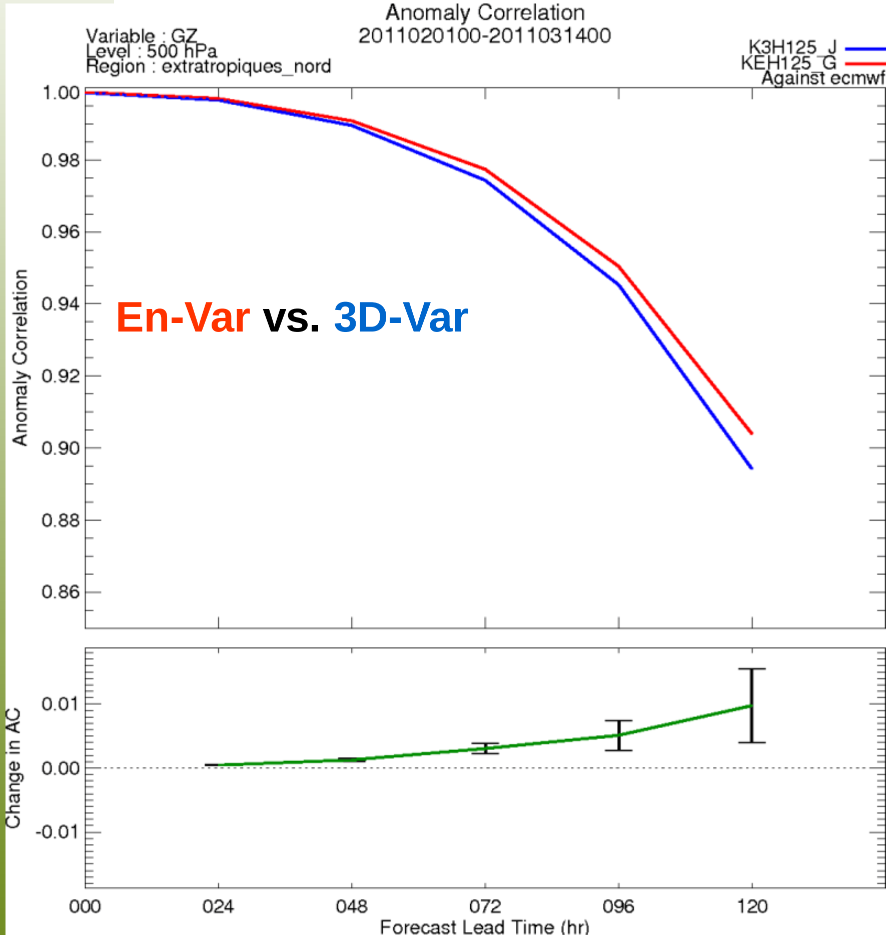
Fairbairn, D., S. R. Pring, A. C. Lorenc and I. R. Roulstone 2012: A comparison of 4D-Var with ensemble data assimilation methods. *Quart. J. Roy. Met. Soc.*, **submitted**

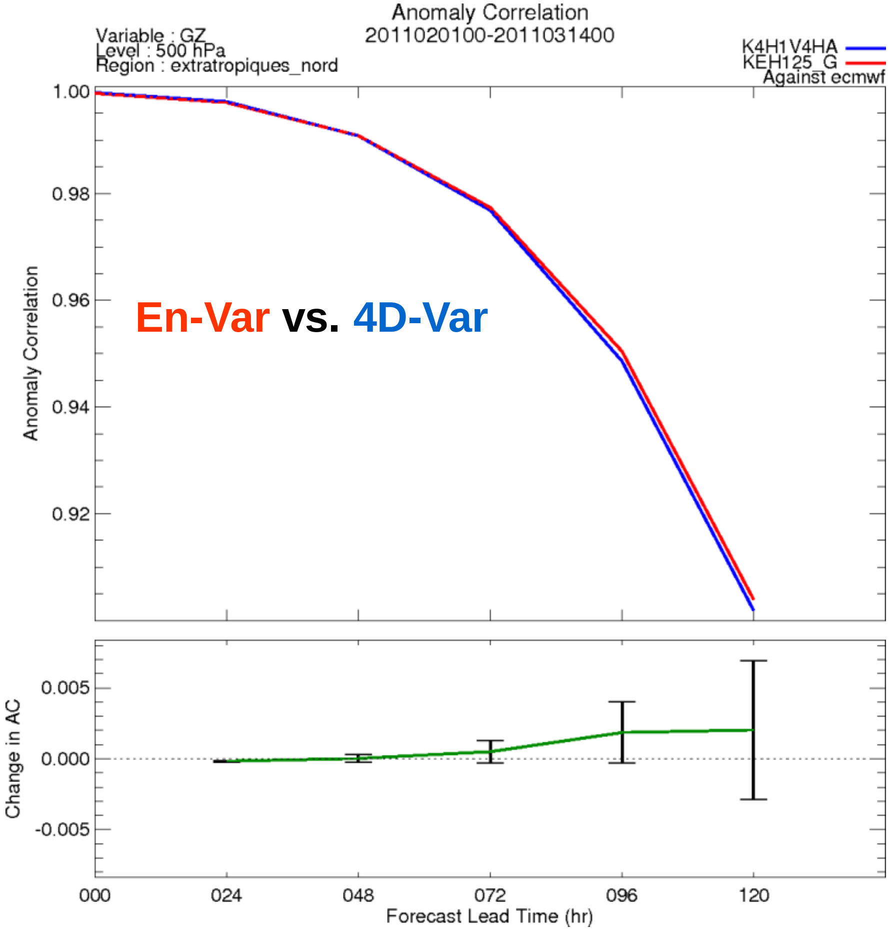


Forecast Results: En-Var vs. 3D-Var and 4D-Var

Verification against ERA-Interim analyses – 6 weeks, Feb/Mar 2011

North extra-tropics
500hPa GZ correlation anomaly

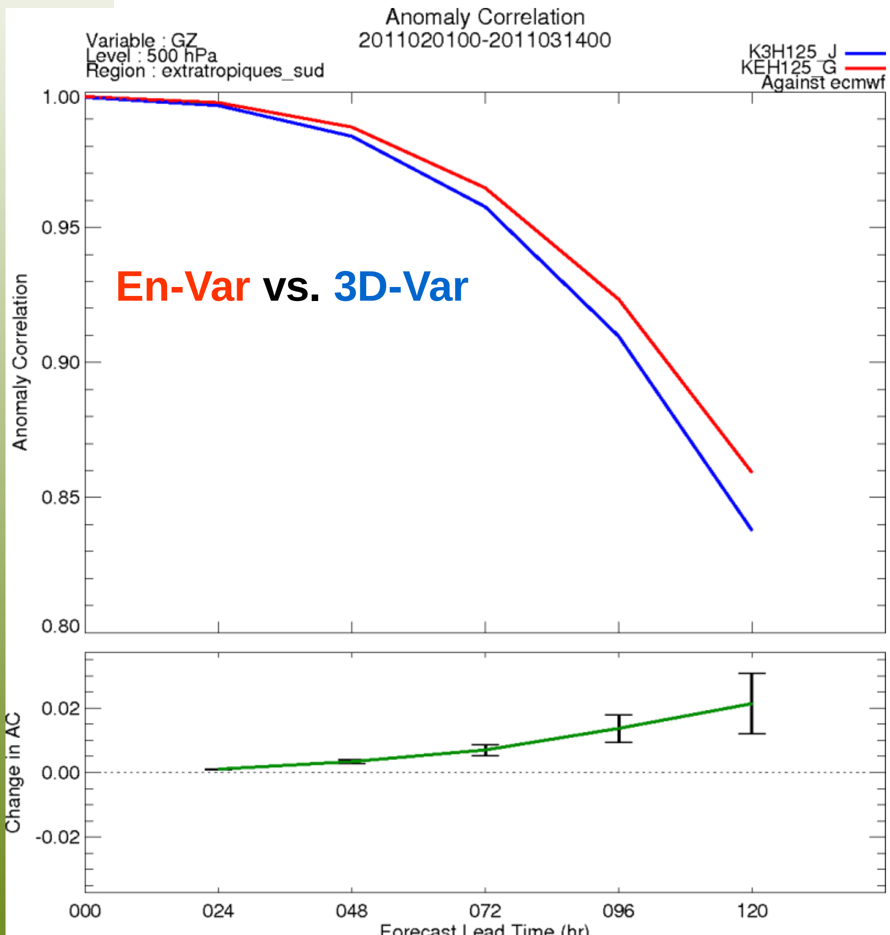


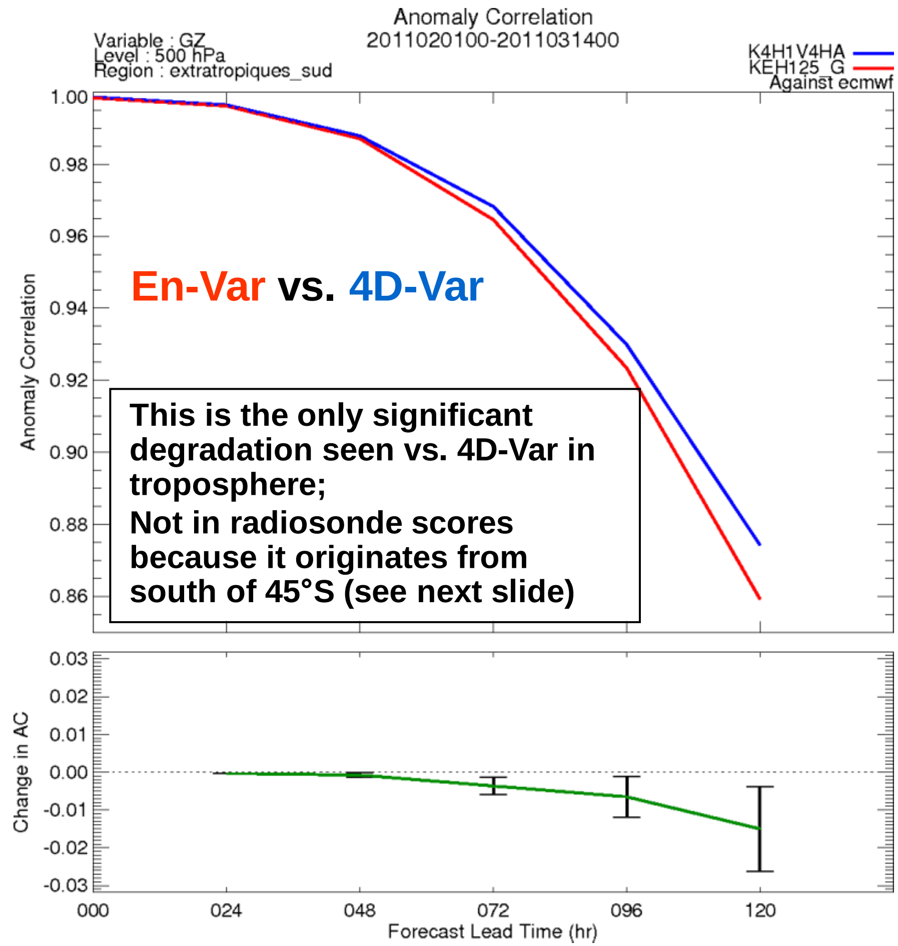


Forecast Results: En-Var vs. 3D-Var and 4D-Var

Verification against ERA-Interim analyses – 6 weeks, Feb/Mar 2011

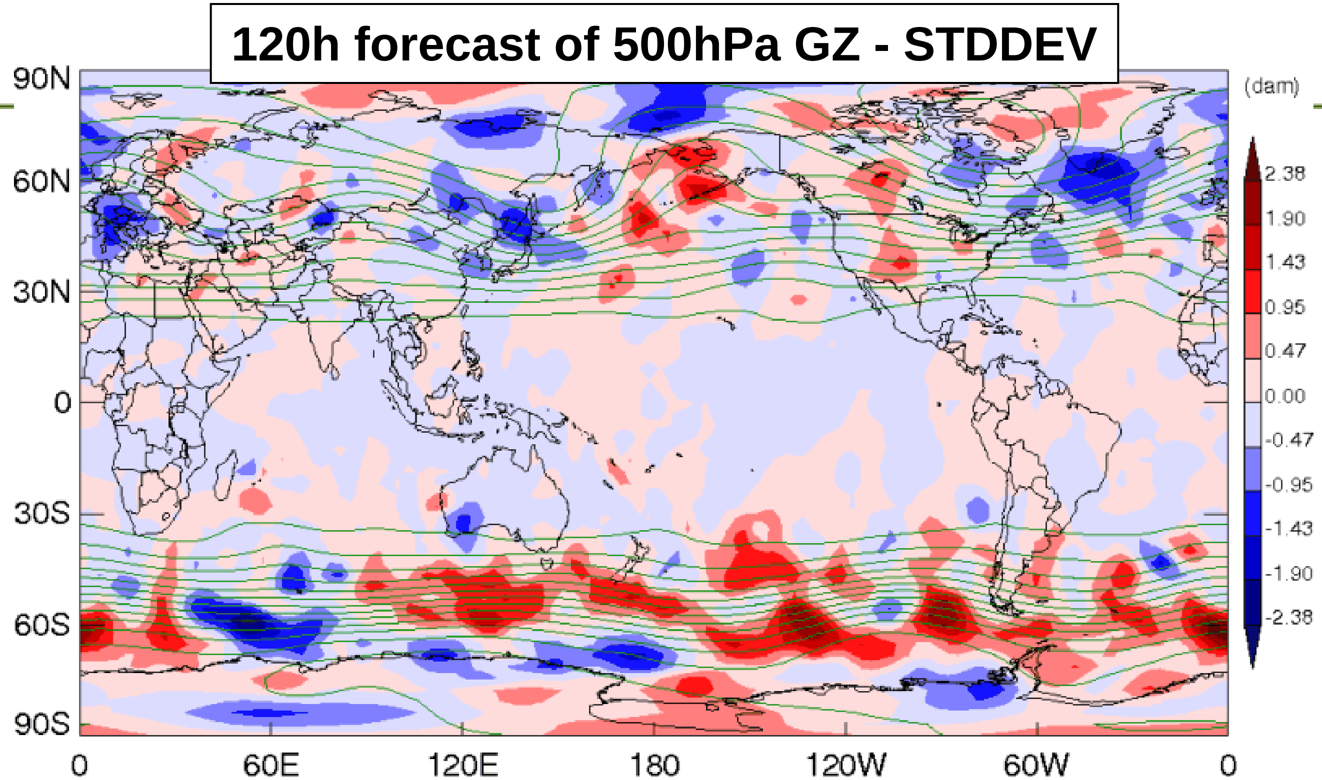
South extra-tropics
500hPa GZ correlation anomaly

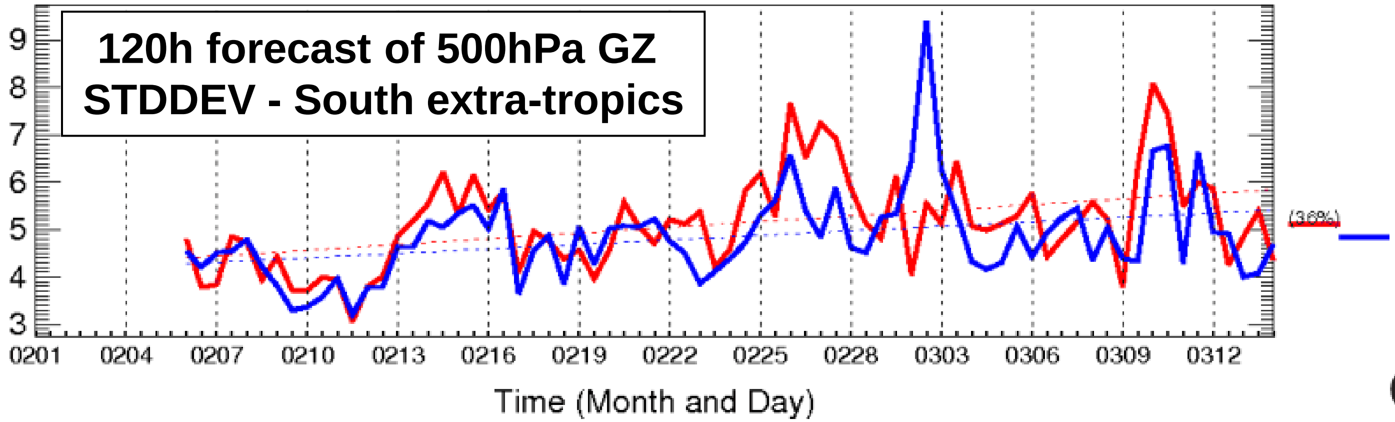




Forecast Results: En-Var vs. 3D-Var and 4D-Var

Verification against ERA-Interim analyses – 6 weeks, Feb/Mar 2011



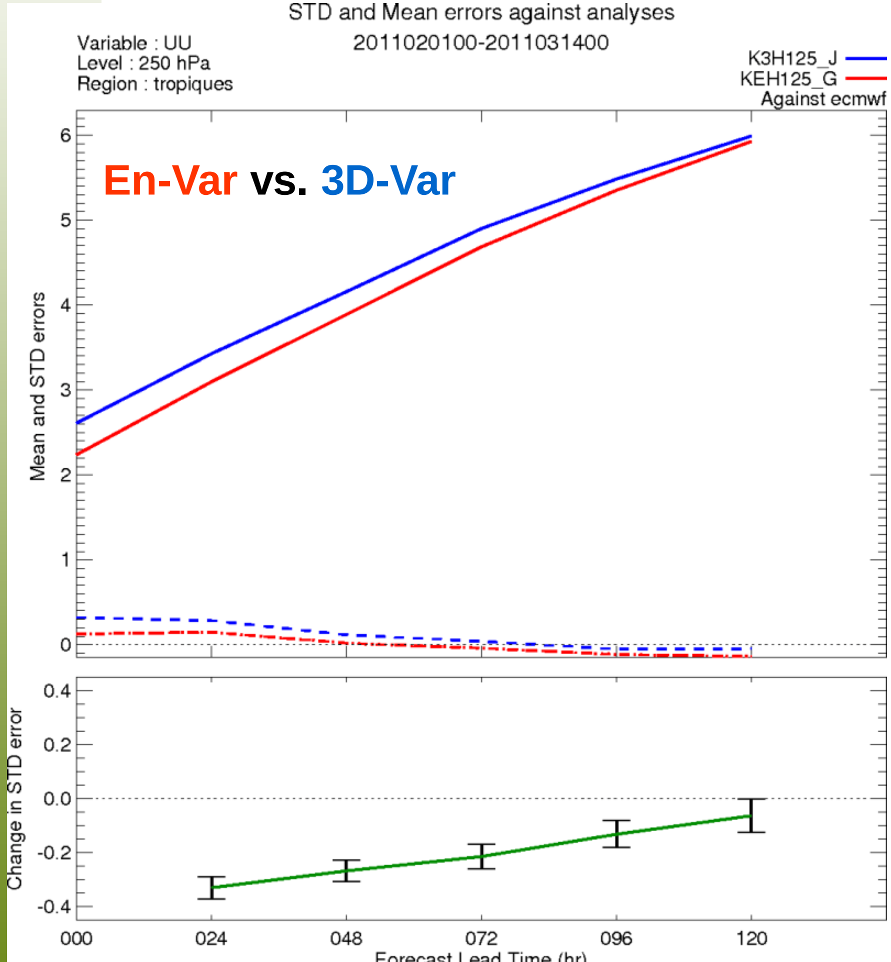


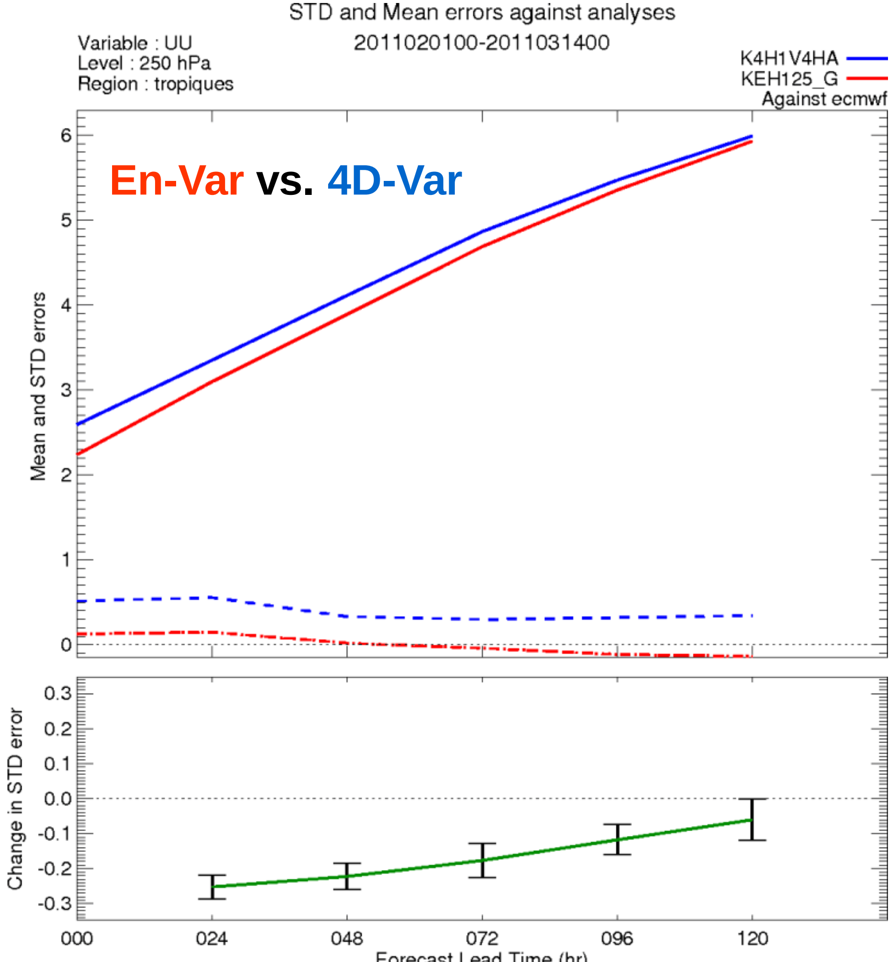
Canada

Forecast Results: En-Var vs. 3D-Var and 4D-Var

Verification against ERA-Interim analyses – 6 weeks, Feb/Mar 2011

Tropics
250hPa U-wind STDDEV

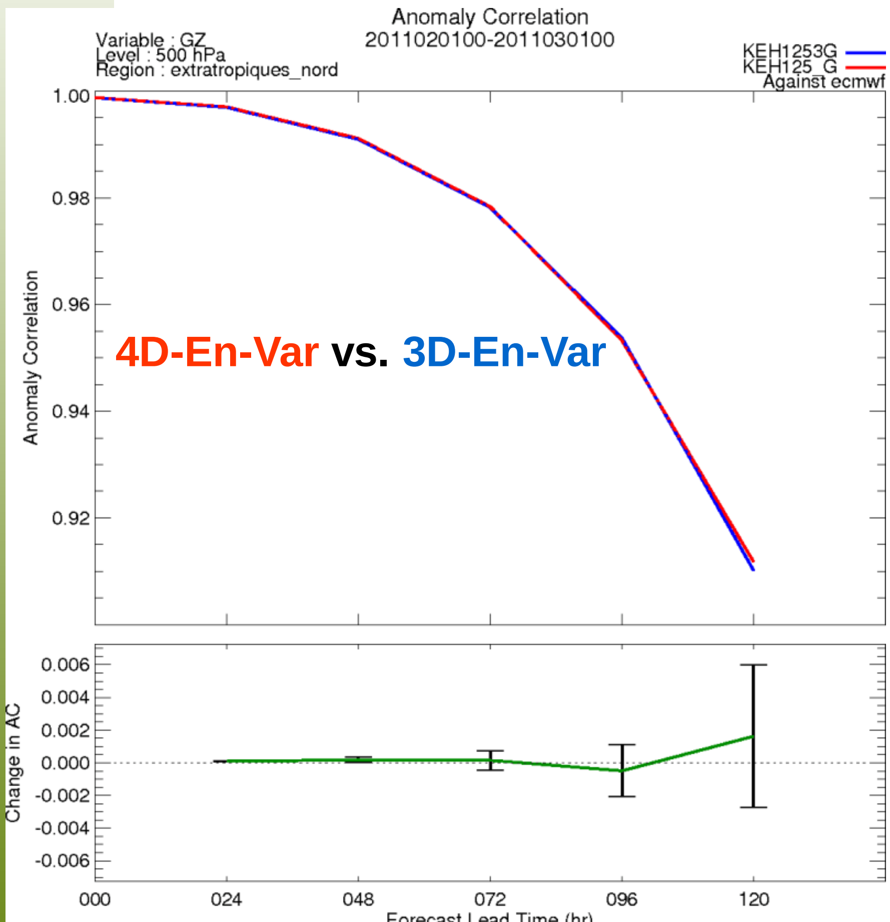


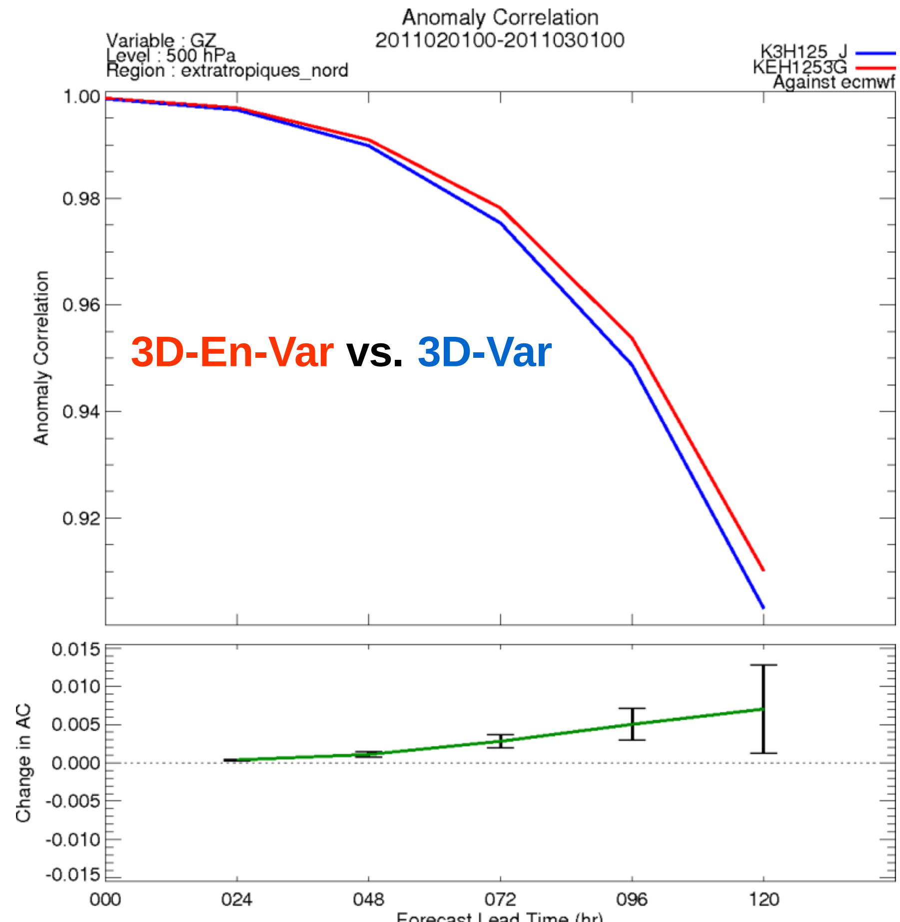


Forecast Results: 4D-En-Var vs. 3D-En-Var

Verification against ERA-Interim analyses – 4 weeks, Feb 2011

North extra-tropics
500hPa GZ correlation anomaly

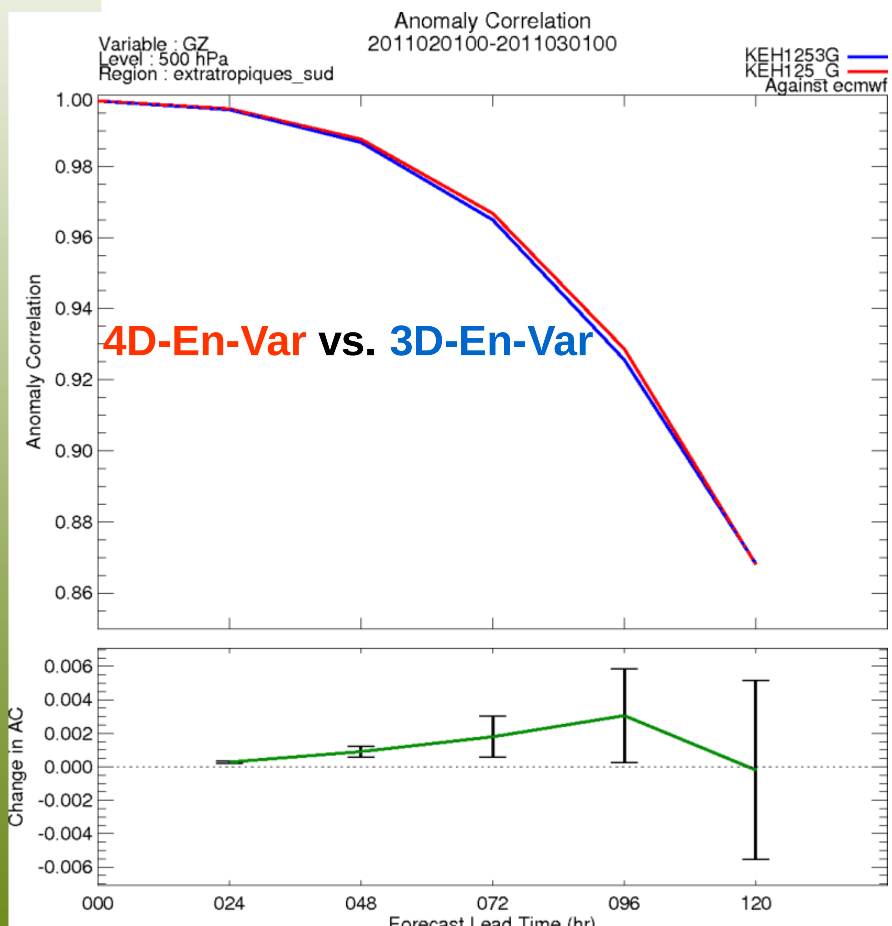


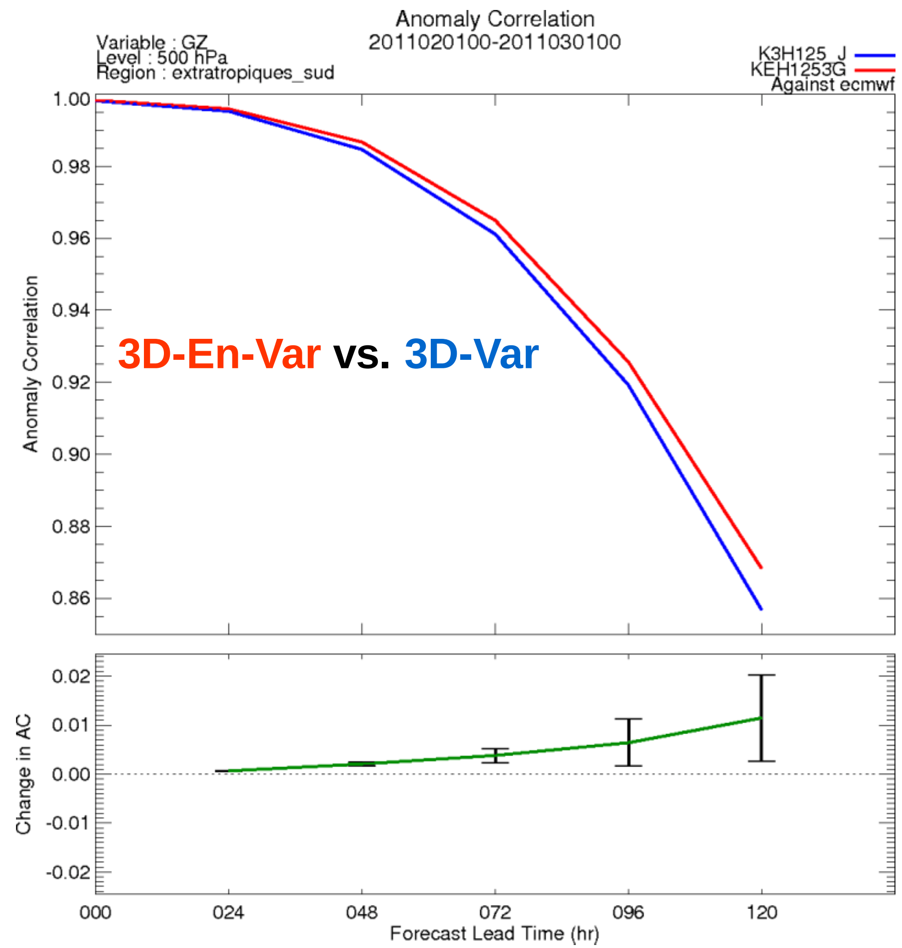


Forecast Results: 4D-En-Var vs. 3D-En-Var

Verification against ERA-Interim analyses – 4 weeks, Feb 2011

South extra-tropics
500hPa GZ correlation anomaly

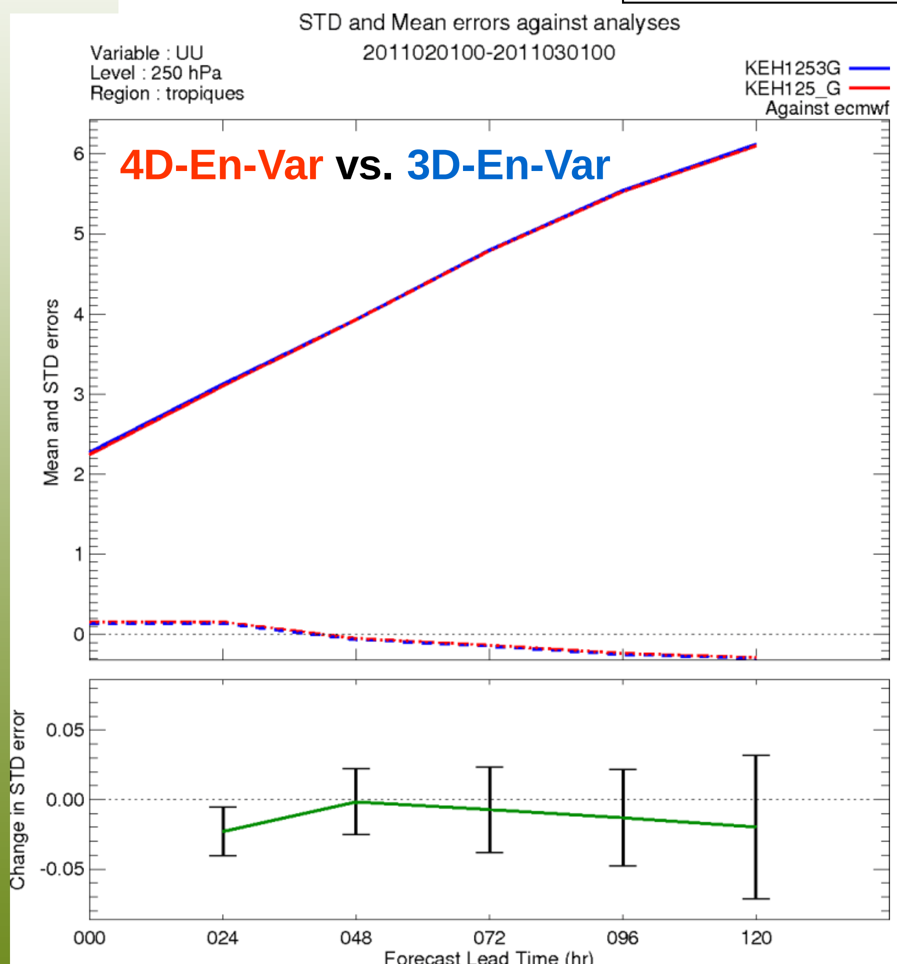


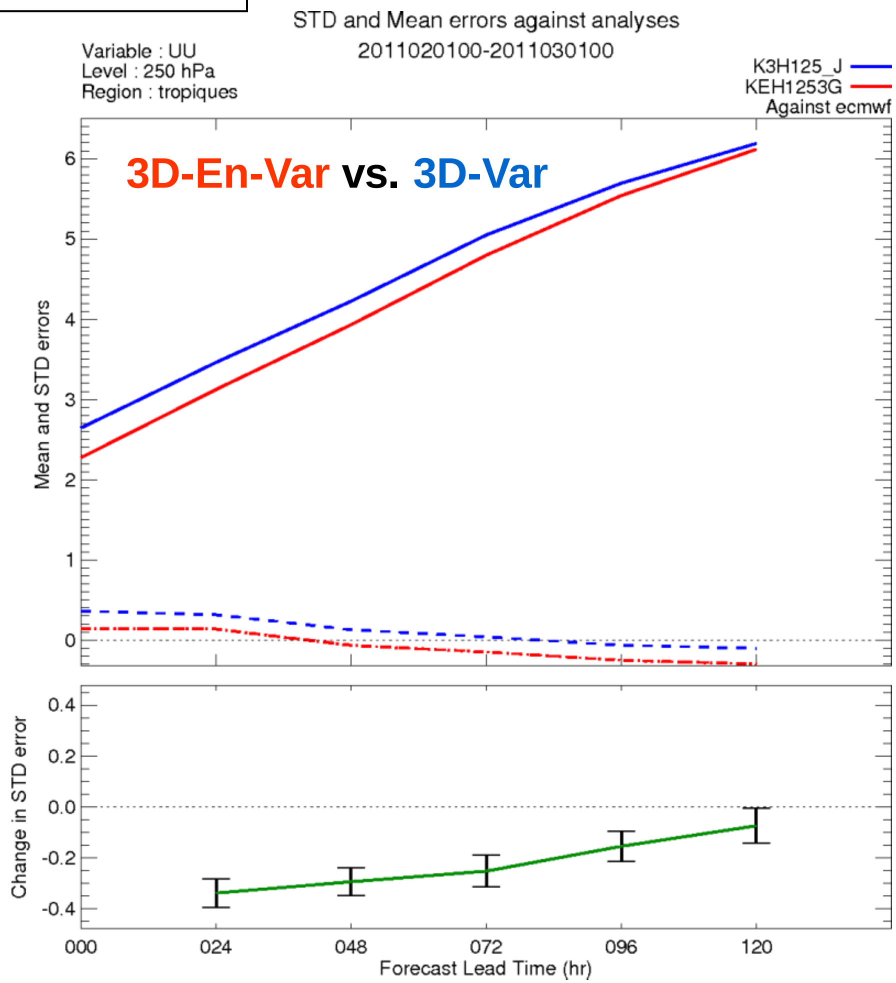


Forecast Results: 4D-En-Var vs. 3D-En-Var

Verification against ERA-Interim analyses – 4 weeks, Feb 2011

Tropics
250hPa U-wind STDDEV





Met Office 4D-En-Var system - Implementation

- Reads ensemble, calculates perturbations, transforms variables, waveband filters (30% + memory)
- Each iteration cost 10% of 4D-Var (N216, 6hr)
- Can process an ensemble of minimisations in one run, to save preprocessing costs and facilitate inflation calculations.
- Trials starting.

Met Office 4D-En-Var system - Plans

- Do not expect it to beat the operational hybrid 4D-Var – It is a contingency against one of the following:
  - new model with no adjoint;
  - new massively parallel computer;
  - need for running-cost savings, e.g. to spend on outerloop or higher resolution;
  - new implementation, e.g. for frequent rapid runs to provide BCs for UK model.
- Interesting possibilities for UK model – need much research.
- An ensemble of 4D-En-Var might beat operational localETKF (but cost tbd).

NCEP (Daryl)

- In terms of the GDAS, we have several things we are working towards, including:
  1. Extension to 4D-En-Var (similar to UKMO and Canada) or 4D-Hybrid (non TL/AD). There have already been some preliminary experiments completed using an OSSE (part of my PhD research) as well as low-resolution experiments with colleagues at the University of Oklahoma.
  2. Improved localization (perhaps through use of anisotropic filters).
  3. Improved specification of weights between static and ensemble contributions....through ideas proposed by Craig Bishop (I just had a very recent conversation with him about this), scale-dependent weighting (I have some very preliminary results, also from my OSSE-based phd research), or perhaps fully-evolving, flow-dependent weightings (have discussed some ideas on this with Kayo Ide and others).

5. Hybrid covariances – ways of compensating for a small ensemble.

- Clever localisation
  - Spectral (Buehner)
  - Following flow (Bishop)
- Mixing in some climatological **B**
  - Craig Bishop has way of determining weights.
  - Better at allowing “new directions” - model error.
- Increase ensemble size
  - Lagged ensemble
  - Is it important to have an EnKF based ensemble?

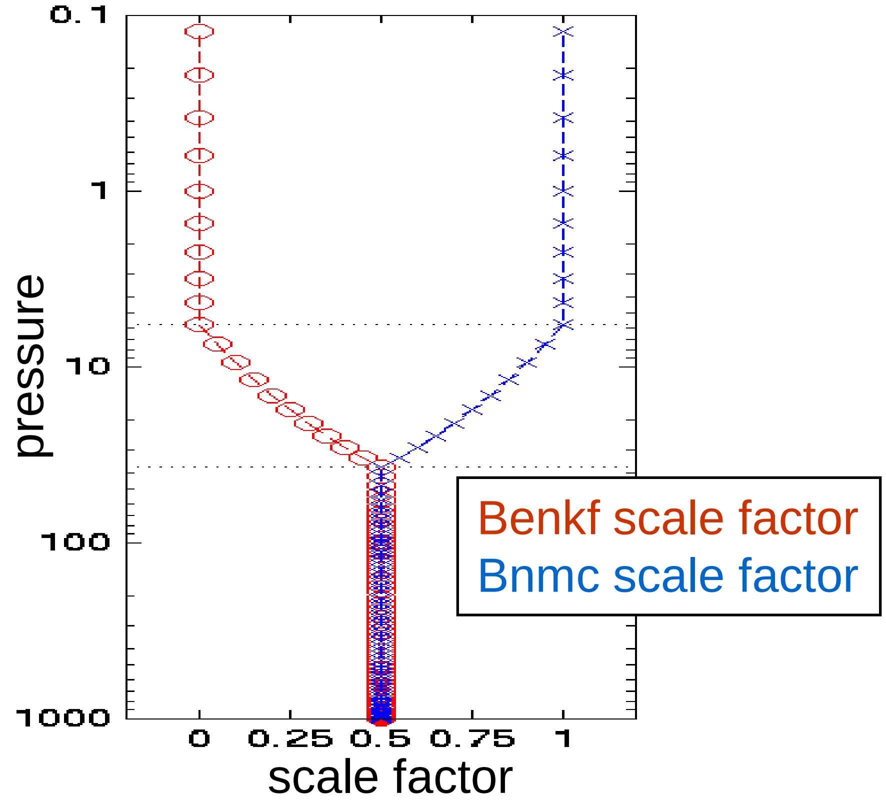
En-Var uses Averaged Covariance Matrix

Model top of EnKF is lower than GDPS

Benkf and Bnmc are averaged in troposphere ½ & ½, tapering to 100% Bnmc at and above 6hPa (EnKF model top at 2hPa)

Therefore, En-Var not expected to be better than 3D-Var above ~10-20hPa

Also tested 75% Benkf and 25% Bnmc in troposphere, but results slightly worse



6. How to generate the ensemble – a separate EnKF or an ensemble of VARs.

- EnKF algorithms are normally less expensive since they only (implicitly) calculate **K** once.
- There is an advantage in generating ensemble & hence covariances using same method as best DA.
- The ensemble size needed for time-varying covariance estimation is much larger than that needed for ensemble forecasting.
- Can centres afford to maintain separate ensemble and "deterministic" systems?

Some examples

Canada: considering using En-Var to cycle 20 additional members (in addition to our 192-member EnKF) that will be used to initialize our 20-member medium-range ensemble forecast, using the 192-member EnKF for the covariances, like for the deterministic analysis - I don't think it will be feasible to have a large ensemble of VARs - the EnKF is incredibly efficient!

Met Office: current 40-member ETKF system for perturbations only, centred on 4D-Var. Few R&D resources so will consider ensemble of 4D-En-Var (deterministic rather than perturbed obs).

NCEP: 80 member EnKF (working on consolidation with ETR (bred vector) based system).

ECMWF: EDA small (10) ensemble of low-resolution perturbed observation 4D-Var.

Météo-France: small ensemble of low-resolution perturbed observation 4D-Var.

7. Terminology

Suggestions based on usual current usage.

hybrid applies to covariance, not method. E.g. "hybrid 4D-Var"

EnKF, ETKF, etc generate ensembles

3D-Var, 4D-Var, EnVar, etc generate a single best estimate, unless specified e.g. "An ensemble of 4D-Vars"

4D-Var **<u>always</u>** uses a forecast model and adjoint to generate time−covariances

4D-EnVar, 4DEnKF, etc use the ensemble to generate time−covariances. (The 4D may be omitted)

—   in 4D-Var, 3D-Var was standardised by Ide et al 1997 (and QJ), but not elsewhere. It may be omitted in new names.

7 continued. Some contentious examples

4D-Var-Ben or **En-4D-Var** are 4D-Var with an ensemble covariance (but En-4D-Var has been used differently).

hybrid-4D-Var or **4D-Var-Bhybrid** are 4D-Var with a hybrid covariance. How do we differentiate ECMWF's and Met Office's hybrid 4D-Var?

hybrid-4D-EnVar is a hybrid of a 3D climatological and a 4D−En covariance. (I am developing an "**ensemble of hybrid-4D-EnVar**". The "hybrid" can be omitted.)

hybrid-EnKF could be EnKF with additive inflation sampled from a climatological B. The "hybrid" is omitted by Houtekamer & Mitchell.