



4D-Ensemble-Var – a development path for data assimilation at the Met Office

Probabilistic Approaches to Data Assimilation for Earth Systems,
BIRS, Banff, February 2013.

Andrew Lorenc



Outline of Talk

- Why are we doing it? What is wrong with 4D-Var?
Why do we need an ensemble?

- Addressed by:

Hybrid-4D-Var. Flow-dependent covariances from localised ensemble perturbations.

4DEnVar. No need to integrate linear & adjoint models.

An Ensemble of 4DEnVar. Or alternatives.

- Preliminary results, and plans.



Background

- 4D-Var has been the best DA method for operational NWP for the last decade (Rabier 2005).
- Since then we have gained a day's predictive skill – the forecast “background” is usually very good; properly identifying its likely errors is increasingly important.
- Most of the gain in skill has been due to increased resolution, which was enabled by bigger computers. To continue to improve, we must make effective use of planned massively parallel computers.
- At high resolution, we can no longer concentrate on a single “deterministic” best estimate (Lorenc and Payne 2007); an ensemble sampling plausible estimates is better.



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Outline of 4D-Var

Background \mathbf{x}^b and a transform \mathbf{U} based on the error covariance \mathbf{B} of \mathbf{x}^b

$$\mathbf{U}\mathbf{U}^T = \mathbf{B}$$

Control variable \mathbf{v} which, via transform \mathbf{U} , defines likely corrections $\delta\mathbf{x}$ to \mathbf{x}^b

$$\delta\mathbf{x} = \mathbf{U}\mathbf{v}$$

Prediction \mathbf{y} of observed values \mathbf{y}^o using model $\underline{\mathbf{M}}$ and observation operator H

$$\mathbf{y} = H\left(\underline{\mathbf{M}}\left(\mathbf{x}^b + \delta\mathbf{x}\right)\right)$$

Measure misfit J of incremented state to background and observations

$$J(\mathbf{v}) = \frac{1}{2} \mathbf{v}^T \mathbf{v} + \frac{1}{2} \left(\mathbf{y} - \mathbf{y}^o\right)^T \mathbf{R}^{-1} \left(\mathbf{y} - \mathbf{y}^o\right) + J_c$$

Search for minimum of J , using gradient calculated using adjoint operators

$$\left(\frac{\partial J}{\partial \mathbf{v}}\right) = \mathbf{v} + \mathbf{U}^T \underline{\mathbf{M}}^T \mathbf{H}^T \mathbf{R}^{-1} \left(\mathbf{y} - \mathbf{y}^o\right)$$



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Key weaknesses of 4D-Var

1. Background errors are modelled using a covariance usually assumed to be stationary, isotropic and homogeneous.
2. The minimisation requires repeated sequential runs of a (low resolution) linear model and its adjoint.
3. Minimum-variance estimate is only “best” for near-Gaussians. Cannot handle poorly observed coherent features such as convection.

The Met Office has already addressed 1 in its hybrid ensemble-4D-Var (Clayton et al. 2012).

This talk describes our 4D-EnVar developments attempting to extend this to also address 2, and discusses ensemble approaches to address 3.



Scalability – exploiting massively parallel computers

- 4D-Var requires **sequential** running of a reduced resolution linear PF model and its adjoint. It will be difficult to exploit computers with more (but not faster) processors to make 4D-Var run as fast at higher resolution.
- Improved current 4D-Var algorithms **postpone** the problem a few years, but it will probably return, hitting 4D-Var before the high-resolution forecast models.
- **4DCV 4D-Var can be parallelised** over each CV segment (Fisher 2011), but is difficult to precondition well.
- Ensemble DA methods run a similar number of model integrations in **parallel**. It is attractive to replace the iterated running of the PF model by precalculated ensemble trajectories: **4DEnVar**. Other advantages of VAR can be retained.



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).



Simple Idea – Linear combination of ensemble members

- Assume analysis increments are a linear combination of ensemble perturbations

$$\delta \mathbf{x} = \sum_{i=1}^K (\mathbf{x}_i - \bar{\mathbf{x}}) \alpha_i$$

- Independent α_i implies that covariance of $\delta \mathbf{x}$ is that of the ensemble.
- Allow each α_i to vary slowly in space, so eventually we can have a different linear combination some distance away.
- Four-dimension extension: apply the above to ensemble trajectories:

$$\delta \underline{\mathbf{x}} = \sum_{i=1}^K (\underline{\mathbf{x}}_i - \underline{\bar{\mathbf{x}}}) \alpha_i$$



Hybrid 4D-Var formulation

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

$$\mathbf{B}_c = \mathbf{U}\mathbf{U}^T \qquad \delta\mathbf{x}_c = \mathbf{U}\mathbf{v} = \mathbf{U}_p \mathbf{U}_v \mathbf{U}_h \mathbf{v}$$

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

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

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

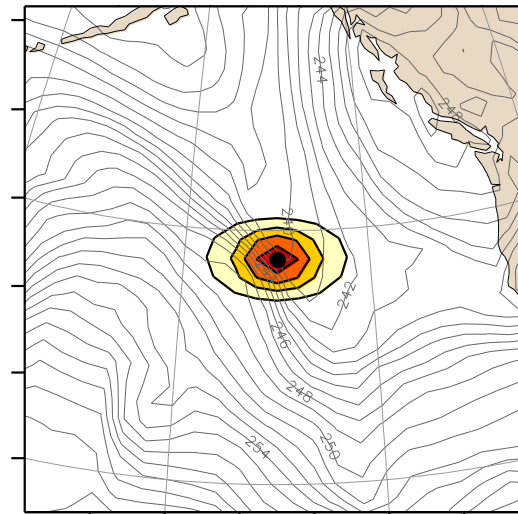
- Hybrid 4D-Var: $\mathbf{y} = H(\underline{\mathbf{M}}(\mathbf{x}_b + \underline{\beta_c} \delta\mathbf{x}_c + \underline{\beta_e} \delta\mathbf{x}_e))$

$$J = \frac{1}{2} \mathbf{v}^T \mathbf{v} + \frac{1}{2} \mathbf{v}^{\alpha T} \mathbf{v}^\alpha + \frac{1}{2} (\mathbf{y} - \mathbf{y}^o)^T \mathbf{R}^{-1} (\mathbf{y} - \mathbf{y}^o) + J_c$$

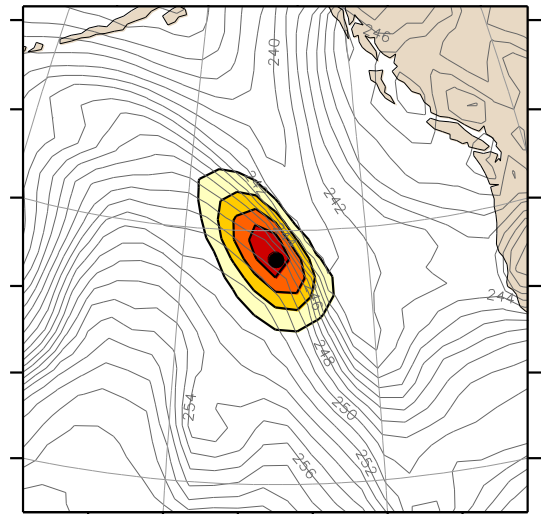
- **Met Office detail:** We localise and combine in transformed variable space to preserve balance and allow a nonlinear \mathbf{U}_p .

u increments fitting a single u ob at 500hPa, at different times.

4D-Var

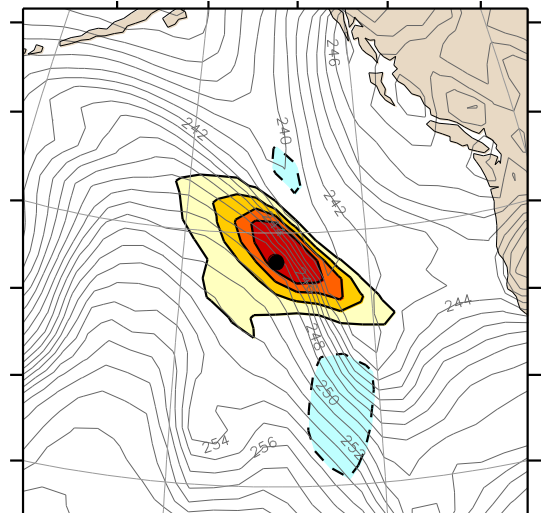
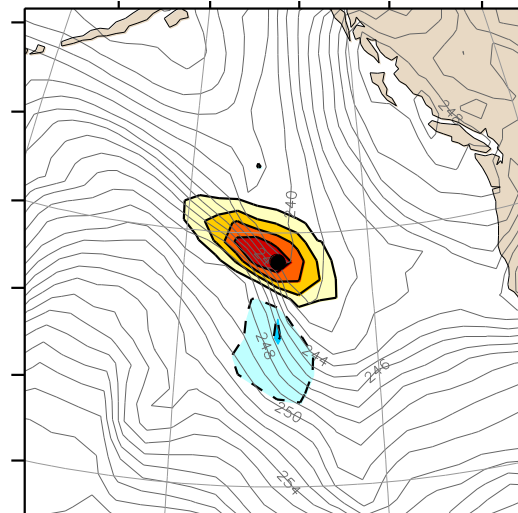


at start of
window



at end of 6-hour
window

Hybrid 4D-Var



Unfilled contours show T field.
Clayton *et al.* 2012

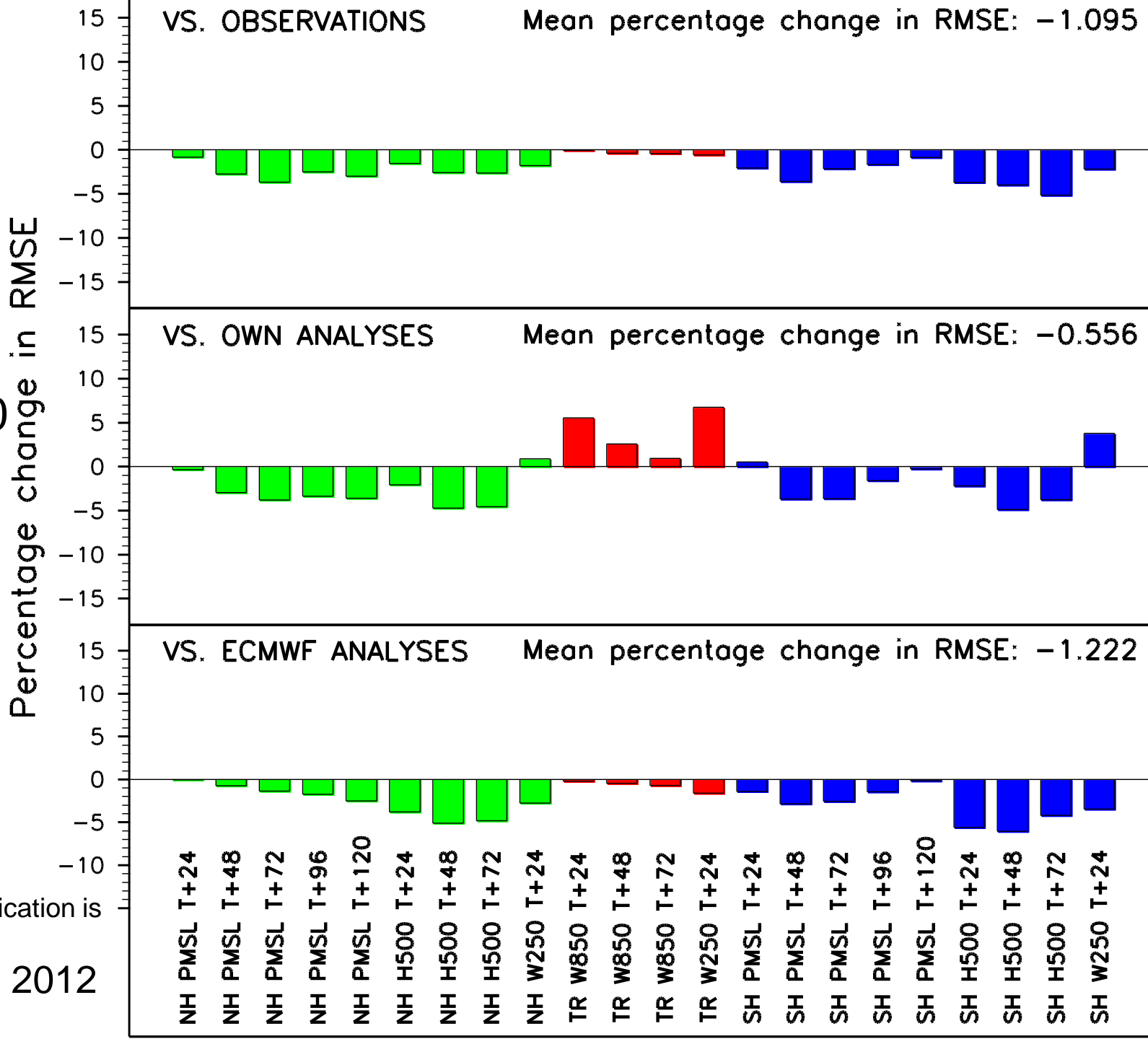


Testing of hybrid 4D-Var

- Used 23 perturbations from operational MOGREPS ensemble system (localised ETKF)
- Straightforward to demonstrate that hybrid-3D-Var performs better than 3D-Var (as in Wang et al. 2008)
- Harder to demonstrate that hybrid-4D-Var performs better than operational 4D-Var.
- Modifications and tuning eventually gave a large and widespread benefit.
- Several more improvements being worked on.



Results from June 2010 parallel trial



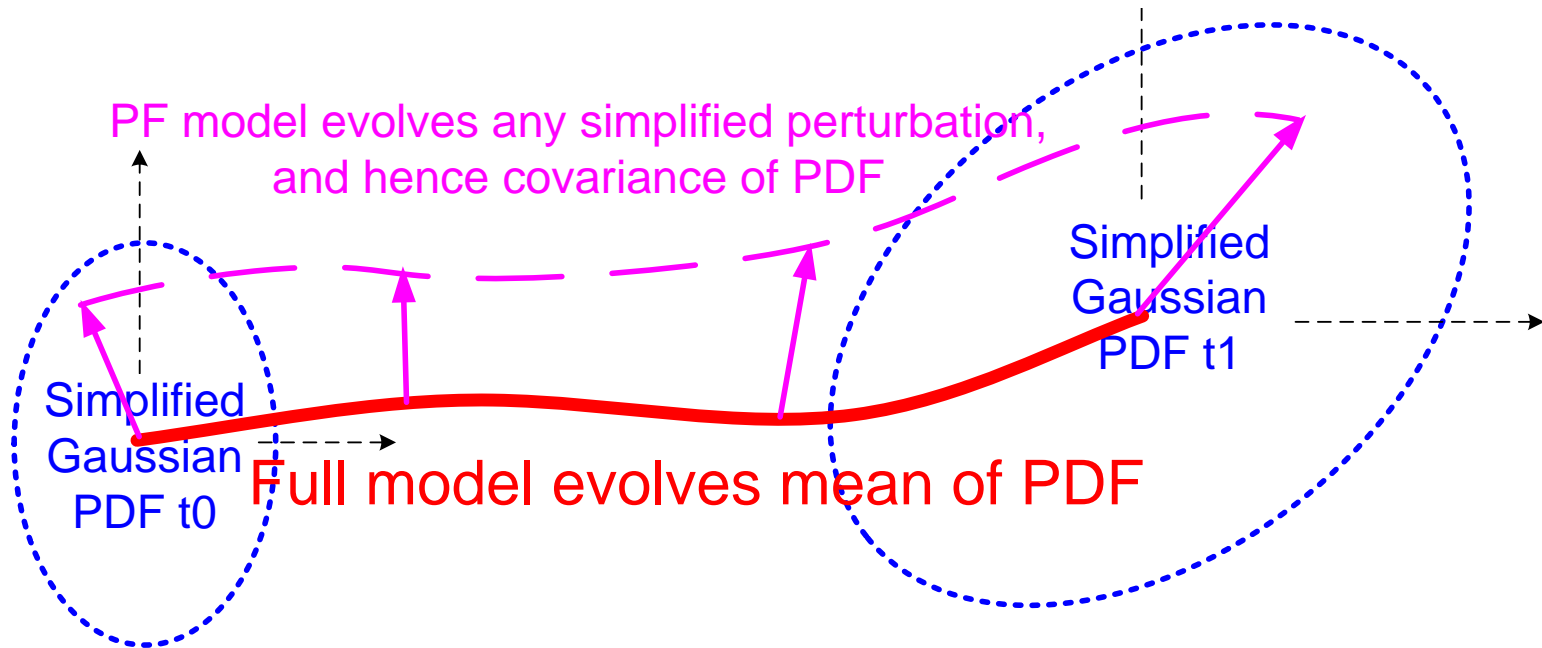
Own Analysis verification is unreliable.
Clayton *et al.* 2012



4D ensemble covariances without using a linear model – 4DEnVar

- Combination of ideas from hybrid-Var 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.

Statistical, incremental 4D-Var

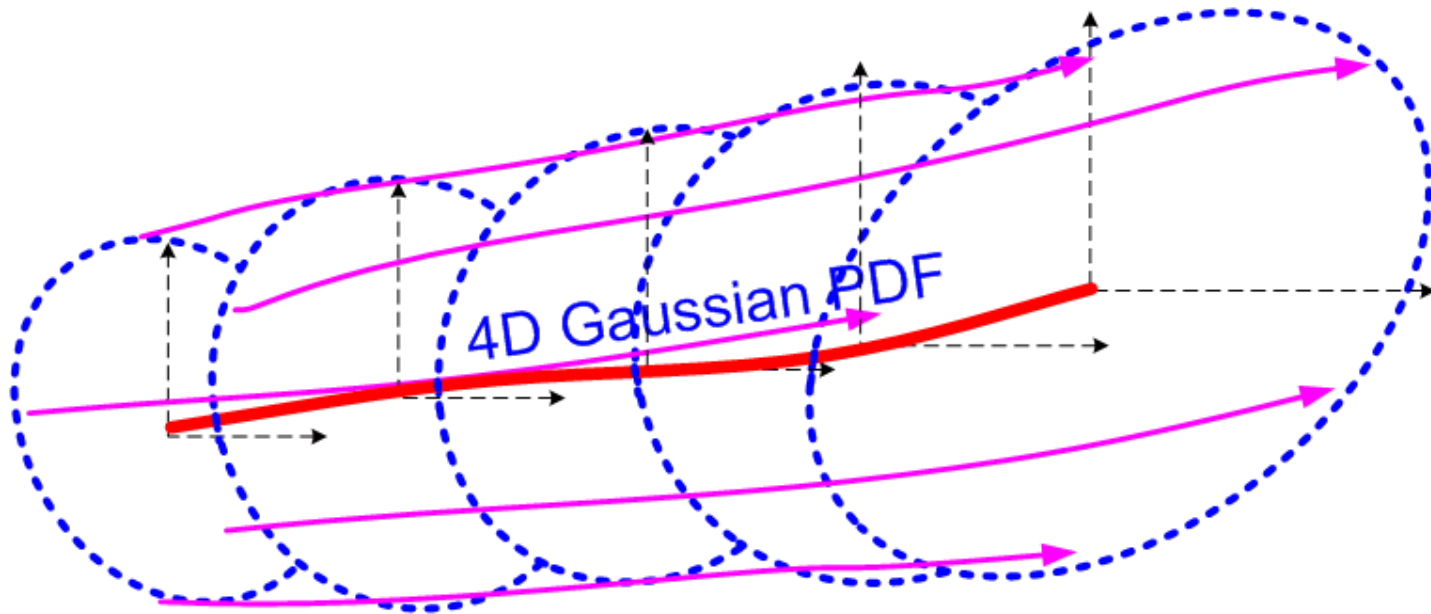


Statistical 4D-Var approximates entire PDF by a 4D Gaussian defined by PF model.

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.



Hybrid 4DEnVar – differences from hybrid-4D-Var

- 4D trajectory is used from background and ensemble, rather than 3D states at beginning of window.

- 4D localisation fields and increment
$$\delta \underline{\mathbf{x}}_e = \frac{1}{\sqrt{K-1}} \sum_{i=1}^K (\underline{\mathbf{x}}_i - \bar{\underline{\mathbf{x}}}) \circ \underline{\mathbf{a}}_i$$

- $\delta \underline{\mathbf{x}}_c$ increment is constant in time, as in 3D-Var FGAT
- No model integration inside minimisation, so costs like hybrid-3D-Var
- No J_c balance constraint, so additional initialisation is necessary.

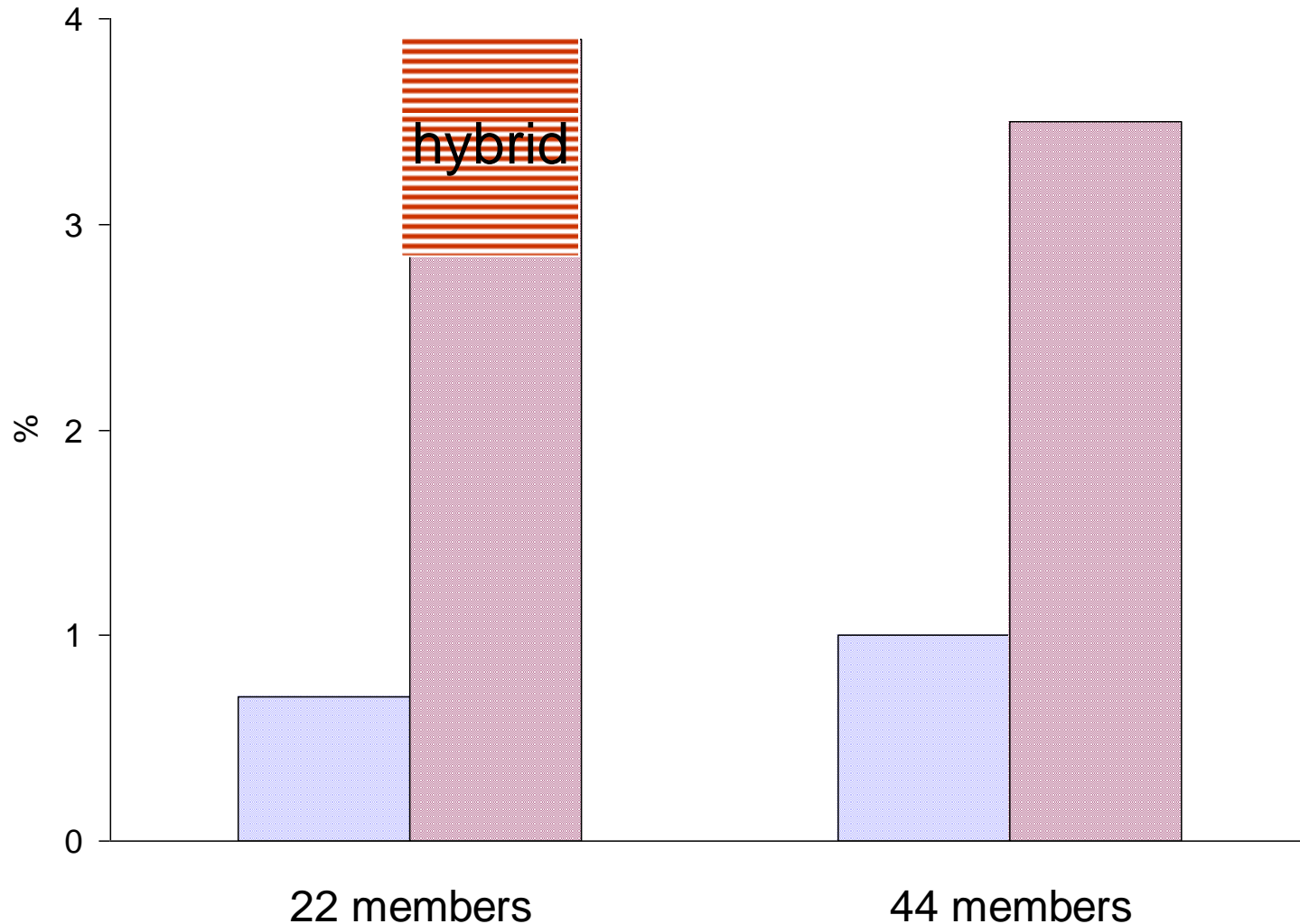
Results of First Trials

- Target is to match operational hybrid-4D-Var
- 4DEnVar was set up with:
 - Same analysis resolution as 4D-Var
 - Same ensemble as hybrid-4D-Var
 - Same climatological \mathbf{B} (but used as in **3D-Var**)
 - Same hybrid β s
 - 100 iterations
 - IAU-like initialisation
- Baseline is hybrid-3D-Var (\approx 3DEnVar)



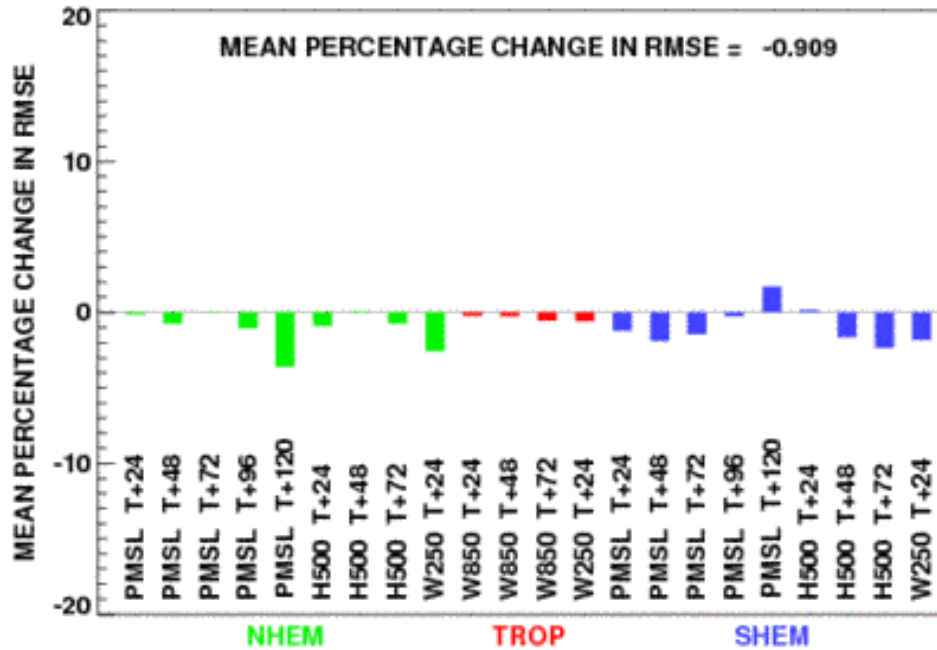
Mean RMS error reduction, compared to hybrid-3D-Var

4D-EnVar hybrid-4D-Var

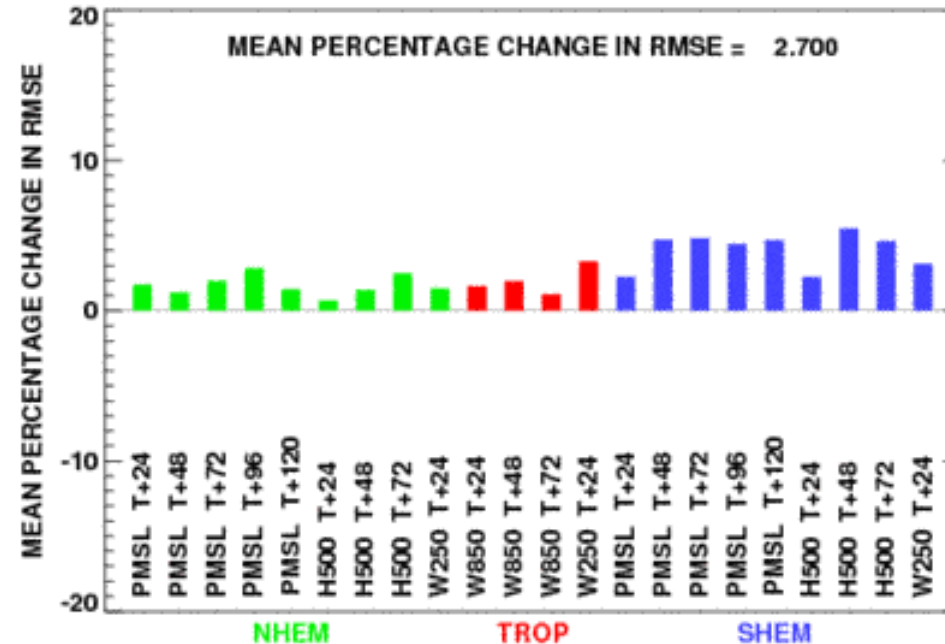




4DEnVar beats hybrid-3D-Var but not hybrid-4D-Var



4DEnVar v hybrid-3D-Var



4DEnVar v hybrid-4D-Var

Verification against observations. 44 members.



4DEnVar is not expected to beat En-4D-Var, all else equal.

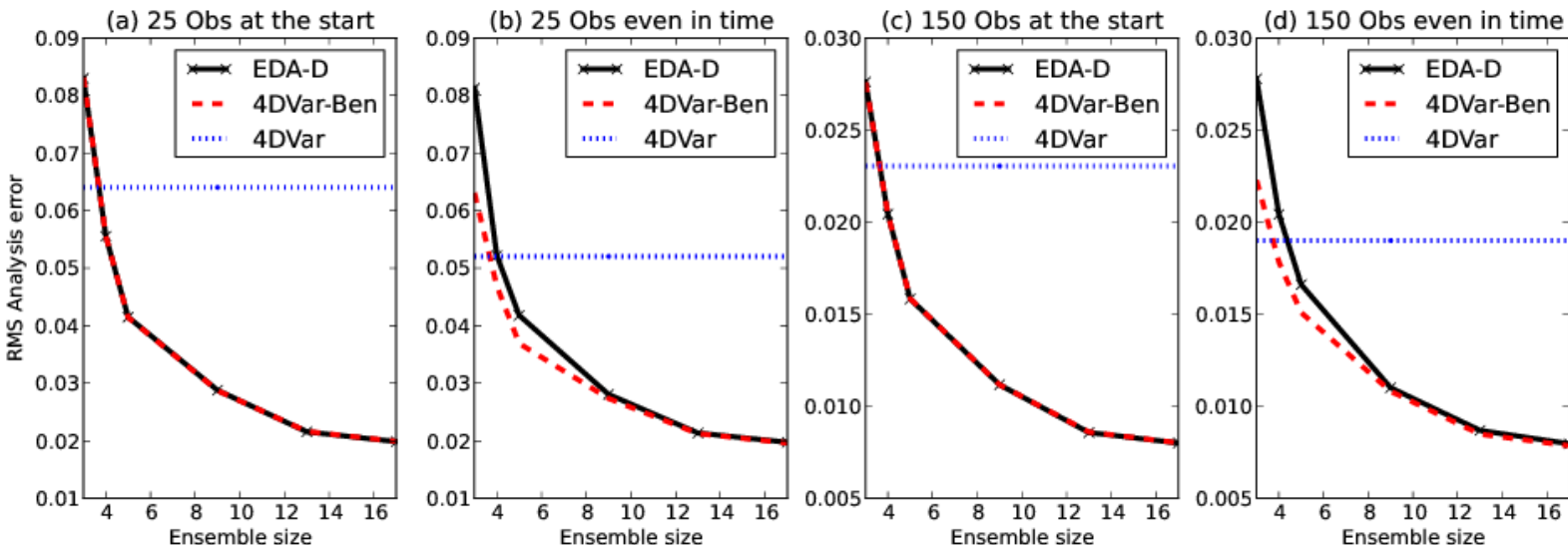
- En-4D-Var uses 4D covariance $\underline{\mathbf{M}}(\underline{\mathbf{L}} \circ \underline{\mathbf{B}}_{ens}) \underline{\mathbf{M}}^T$. Its time-correlations are correct as long as $\underline{\mathbf{M}}$ is accurate.
- 4DEnVar uses perturbations of 4D nonlinear ensemble trajectories from their mean. Ignoring the nonlinearity of the model this equals $\underline{\mathbf{L}} \circ (\underline{\mathbf{M}} \underline{\mathbf{B}}_{ens} \underline{\mathbf{M}}^T)$. Its time-correlations are incorrect because $\underline{\mathbf{L}}$ and $\underline{\mathbf{M}}$ do not commute.
- In spatial dimensions the methods are equivalent.
- Demonstrated in a toy model by Fairbairn *et al.* (2013).



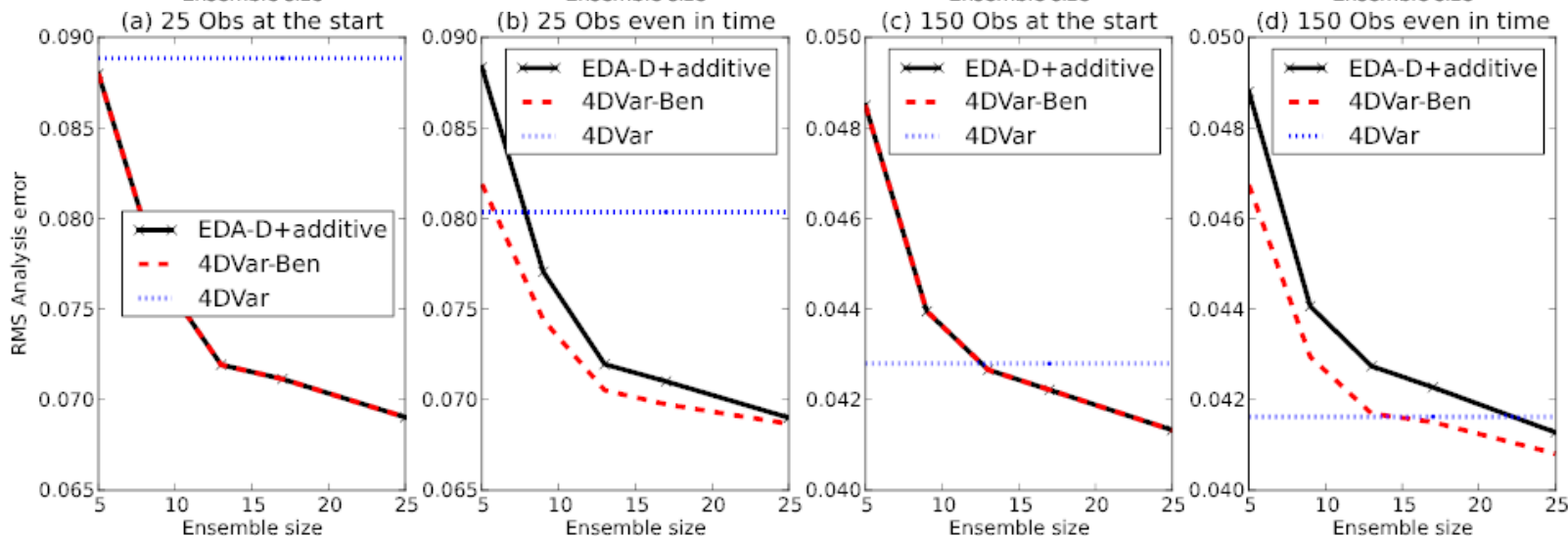
4D-EnVar ν 4D-Var-Ben ν 4D-Var

Toy model results

Perfect model expts.



Imperfect model expts with additive inflation sampled from \mathbf{Q}





The key is in the localisation!

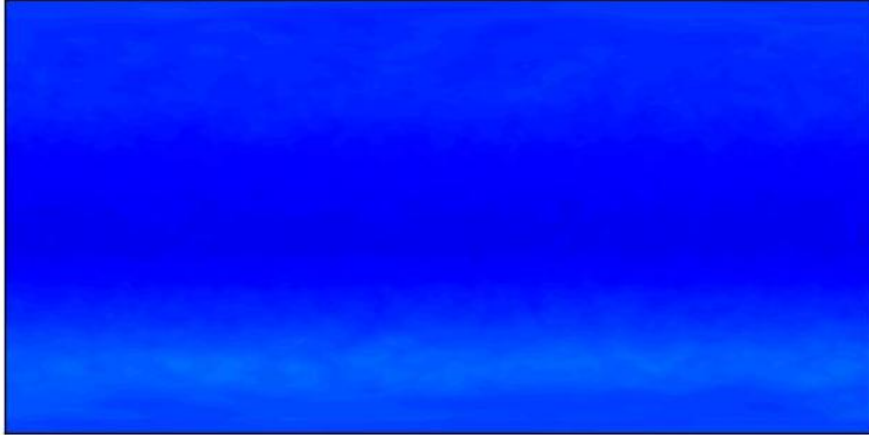
1. Parameter (“balanced” ψ & residuals χ , A_p , μ)
 2. Spectral (Waveband) (Buehner and Charron 2007, Buehner 2012)
 3. Vertical
 4. Horizontal
- Done in the above order – can use this e.g. to apply “balance aware” spatial localisation and to have different horizontal scales for each waveband.
 - Flow following (Bishop and Hodyss 2011)



Spectral localisation smooths in space: σ_b of pressure at level 21

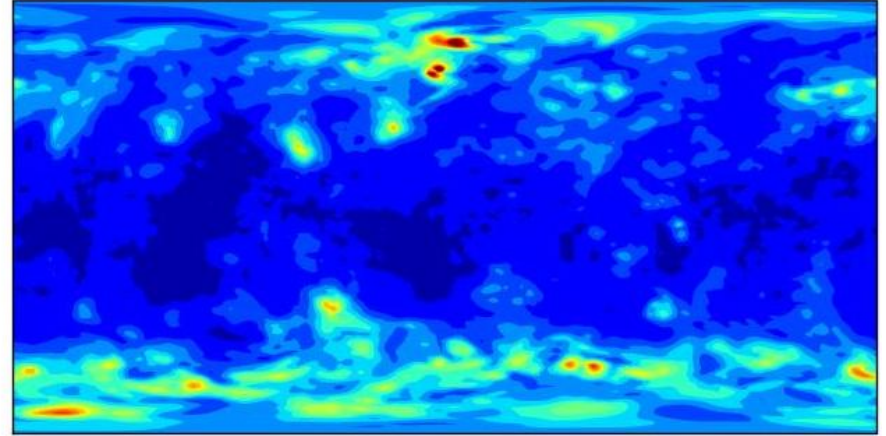
C: Climatological

p: sigma at level 21 3076m, max=46.5911

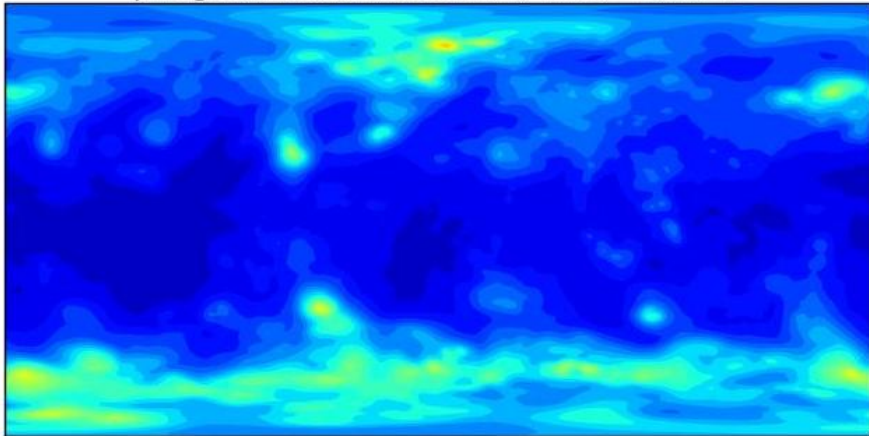


E: Ensemble

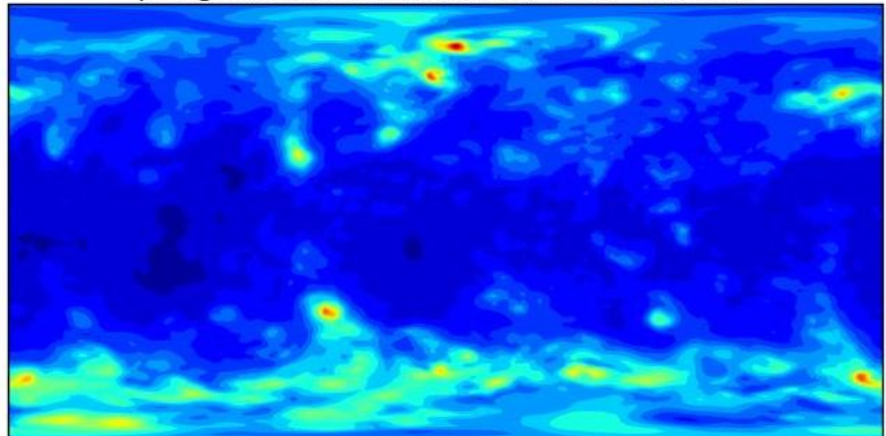
p: sigma at level 21 3076m, max=254.821



locVHhb6IO: Ens + V&varyingH loc + 6 increasing wb, overlap
p: sigma at level 21 3076m, max=141.148



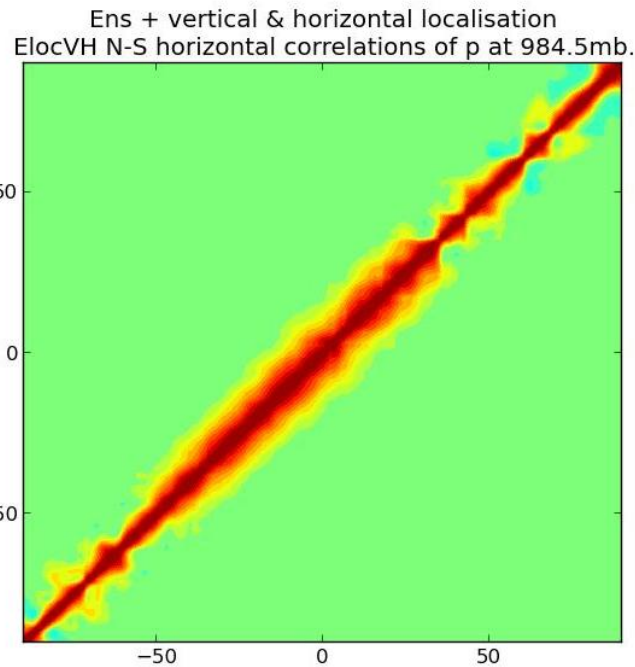
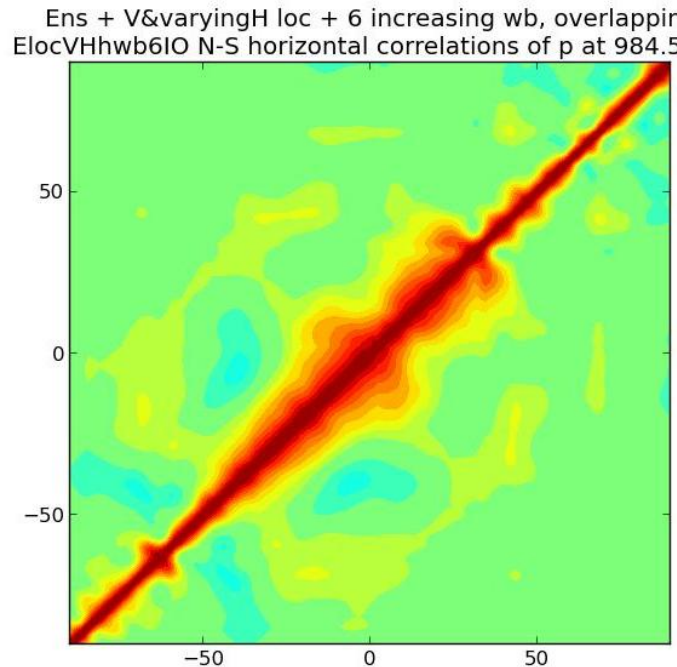
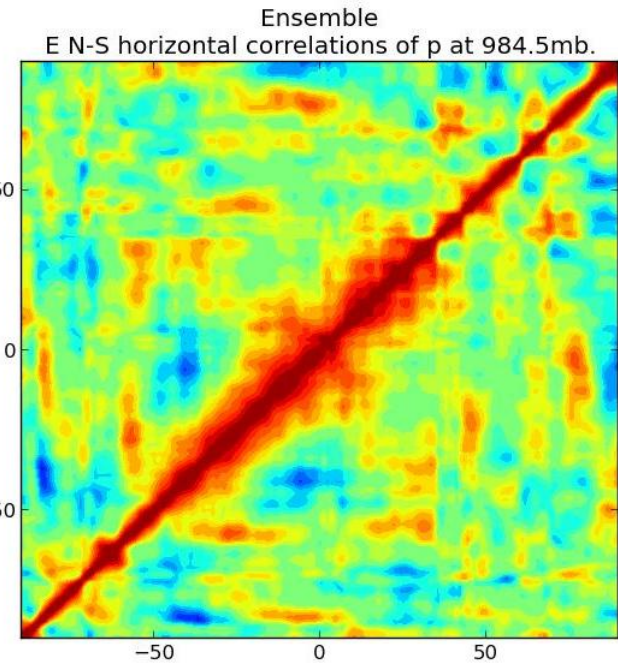
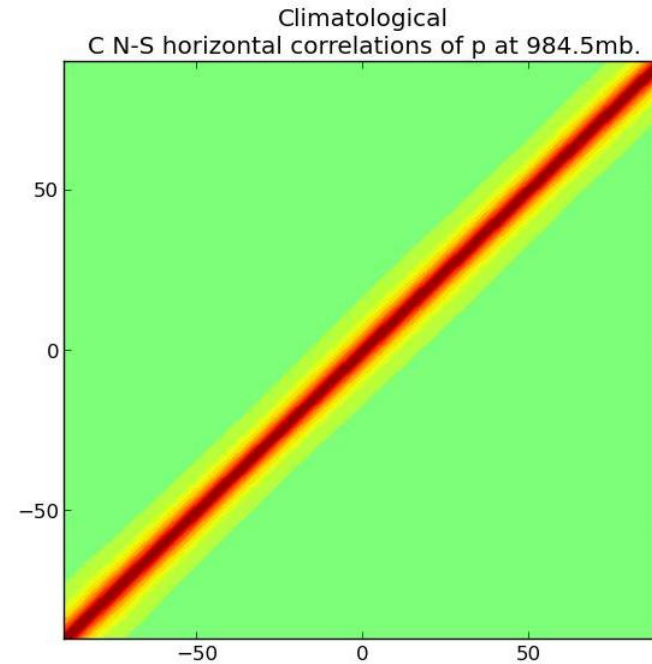
ElocVH: Ens + vertical & horizontal localisation
p: sigma at level 21 3076m, max=197.956





Horizontal correlation along N-S line

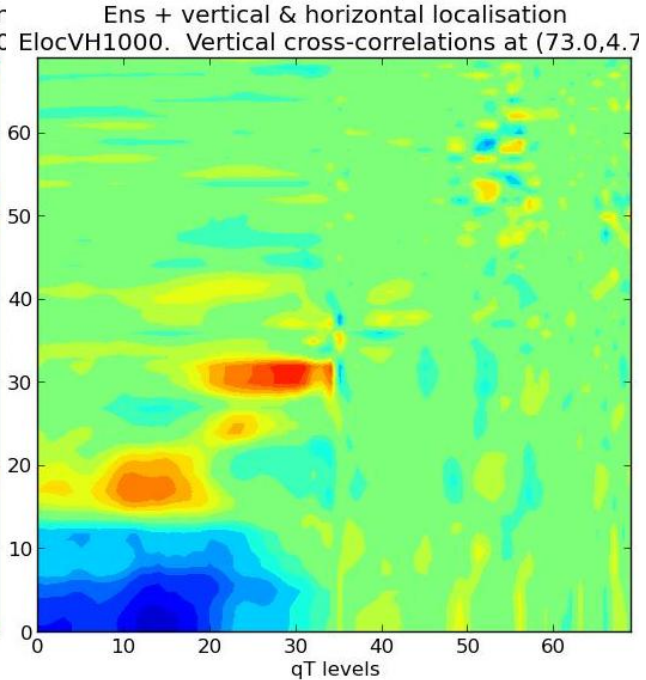
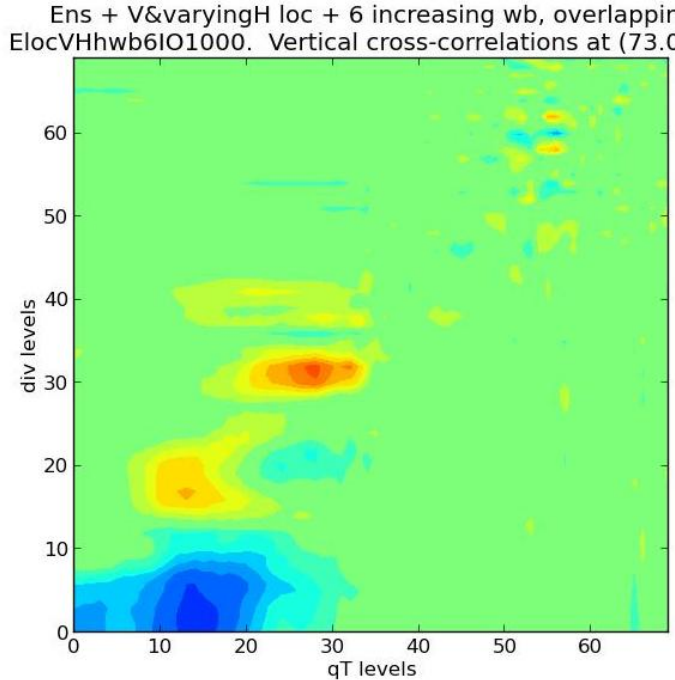
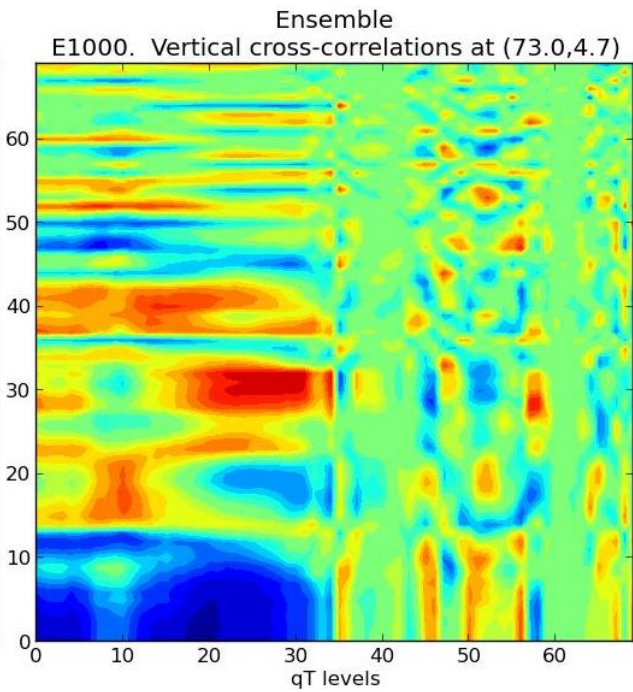
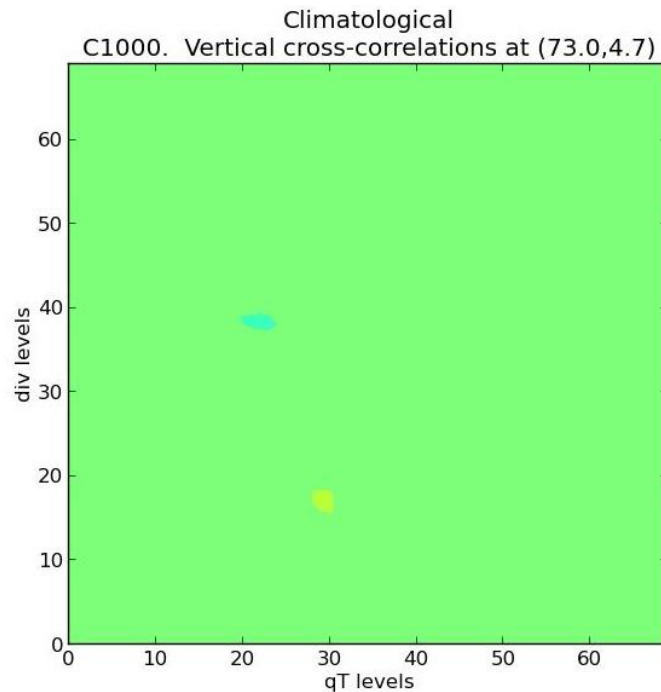
Localisation scales for each waveband seem beneficial





Vertical cross-correlation between q and divergence at an active point.

Localisation (except parameter) retains plausible correlation between q and convergence below, divergence above.





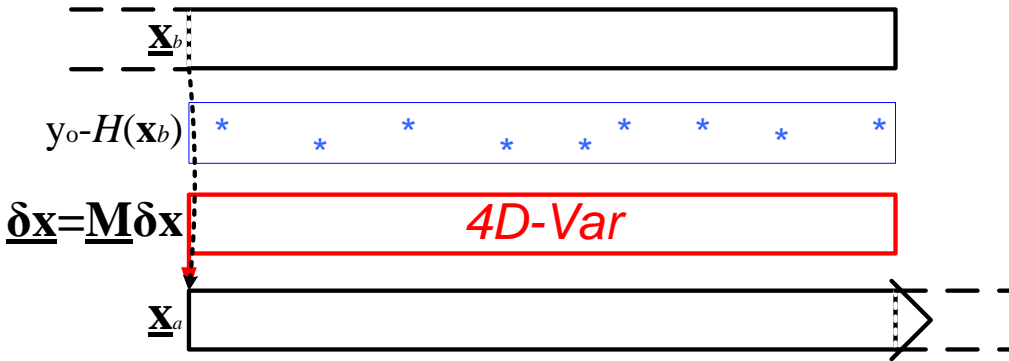
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What is “Best”?

- Minimum-variance Kalman filter based methods such as 4D-Var have enabled big gains in skill we want to keep.
- Regional NWP already represents coherent structures whose position is uncertain.
The ensemble mean is **NOT** a good forecast.
Global models will soon reach such resolutions (5km experiments already).
- Lorenc & Payne (2007) proposed using regularised minimum variance methods for well-known scales. We can rely on the model to develop and maintain fine-scale structure. I.e. the model is making a plausible sample on its attractor from the full, non-Gaussian pdf.
We should have an ensemble of such samples.



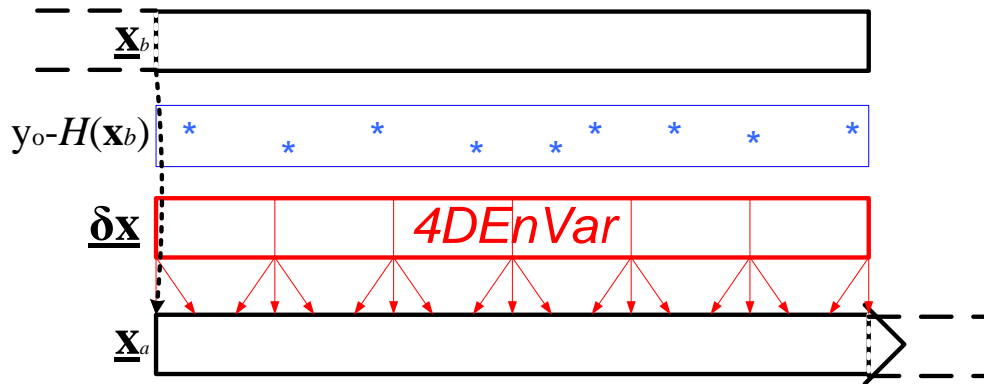
IAU-like interface with forecast model



4D-Var control variables gives initial $\delta\mathbf{x}$, implicitly defining $\underline{\delta\mathbf{x}}$.

$\underline{\delta\mathbf{x}}$ is initialised by Jc term.

Natural to add $\delta\mathbf{x}$ at beginning of forecast; an outer-loop is then easy to organise.



4DEnVar $\underline{\delta\mathbf{x}}$ is defined for all window.

There is no internal initialisation.

Nudge in $\underline{\delta\mathbf{x}}$ during forecast, as part of an IAU-like initialisation. (Bloom *et al.* 1996)

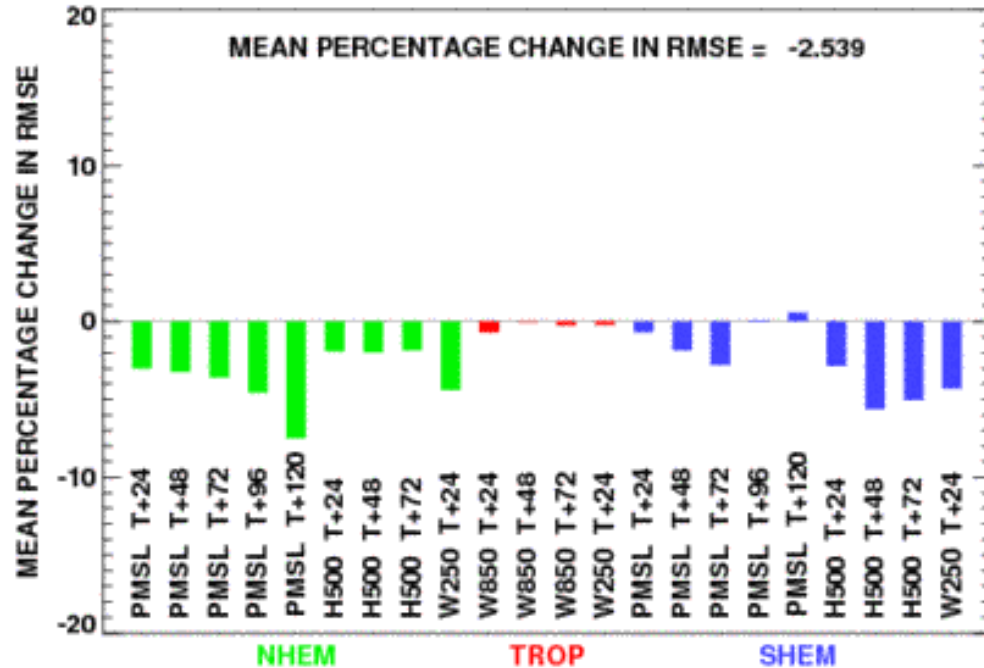


Interface to forecast model has a very large impact on 4D-EnVar.

4D-EnVar with IAU-like interface

v

4D-EnVar with 4D-Var-like interface



(22 member experiments.)



How to generate the ensemble? Alternatives:

1. Separate EnKF. Our current MOGREPS uses a local ETKF (Bowler 2009). It was designed for ensemble forecasting rather than DA.
2. Ensemble of individual 4DEnVar. Worried about IO and memory contention of parallel reads of the ensemble trajectory.
3. Ensemble of 4DEnVar in single executable. Working to reduce run-time cost.
4. EVIL (Tom Augliné). ? Worried about the ability to determine sufficient Hessian eigenvectors.



The differences between ETKF and En4DEnVar in a preliminary experiment

MOGREPS ETKF	En 4DEnVar
Analysis perturbation is added to the deterministic analysis	Analysis Increment is added to each ensemble member's background
Localisation via observation selection in regions	Localisation in model-space (improved balance)
<ul style="list-style-type: none">- Broad horizontal localisation (2000km radius)- No vertical localisation	<ul style="list-style-type: none">- Horizontal localisation with 1200km radius- Vertical localisation



Design Choices for En4DEnVar

- Perturbed obs or DEnKF
- Inflation:
 - Relaxation to prior is already done in DEnKF
 - Adaptive multiplicative, in regions (copied from MOGREPS)
 - Additive. Is this necessary in a hybrid scheme?
 - Stochastic physics and random parameters (copied from MOGREPS)
- Optimisation for massively parallel computer:
 - Add another dimension to domain-decomposition.
 - Combine OpenMP & message-passing.
- Optimisation of algorithm:
 - Independent, or mean & perturbations
 - Preconditioning etc. (Desrozier & Berre 2012)
 - *Avoid En4DEnVar by using EVIL*



DEnKF

ensemble of perturbations

Bowler et al. (2012), inspired by Sakov (2008), showed that a DEnKF can first solve the standard equation for the mean, then a modified equation for the perturbations from the mean, with $\beta \approx 0.5$

$$\bar{x}^a = \bar{x}^f + \mathbf{P}^f \mathbf{H}^T (\mathbf{H} \mathbf{P}^f \mathbf{H} + \mathbf{R})^{-1} (\mathbf{y}^o - H(\bar{x}^f))$$

$$\mathbf{x}'^a = \mathbf{x}'^f - \beta \mathbf{P}^f \mathbf{H}^T (\beta \mathbf{H} \mathbf{P}^f \mathbf{H} + \mathbf{R})^{-1} \mathbf{H} \mathbf{x}'^f.$$

Similar to “relaxation to prior” inflation. Variational equivalent:

$$J(\bar{x}) = \frac{1}{2} (\bar{x} - \bar{x}^f)^T (\mathbf{P}^f)^{-1} (\bar{x} - \bar{x}^f) + \frac{1}{2} (\bar{\mathbf{y}} - \mathbf{y}^o)^T \mathbf{R}^{-1} (\bar{\mathbf{y}} - \mathbf{y}^o)$$

$$\bar{\mathbf{y}} = H(\bar{x}^f + \delta \bar{x})$$

$$J(\delta \mathbf{x}_k) = \frac{1}{2} (\delta \mathbf{x}_k - \delta \bar{x})^T (\beta \mathbf{P}^f)^{-1} (\delta \mathbf{x}_k - \delta \bar{x}) + \frac{1}{2} (\mathbf{y}_k - \bar{\mathbf{y}})^T \mathbf{R}^{-1} (\mathbf{y}_k - \bar{\mathbf{y}})$$

$$\mathbf{y}_k = H(\mathbf{x}_k^f + \delta \mathbf{x}_k)$$



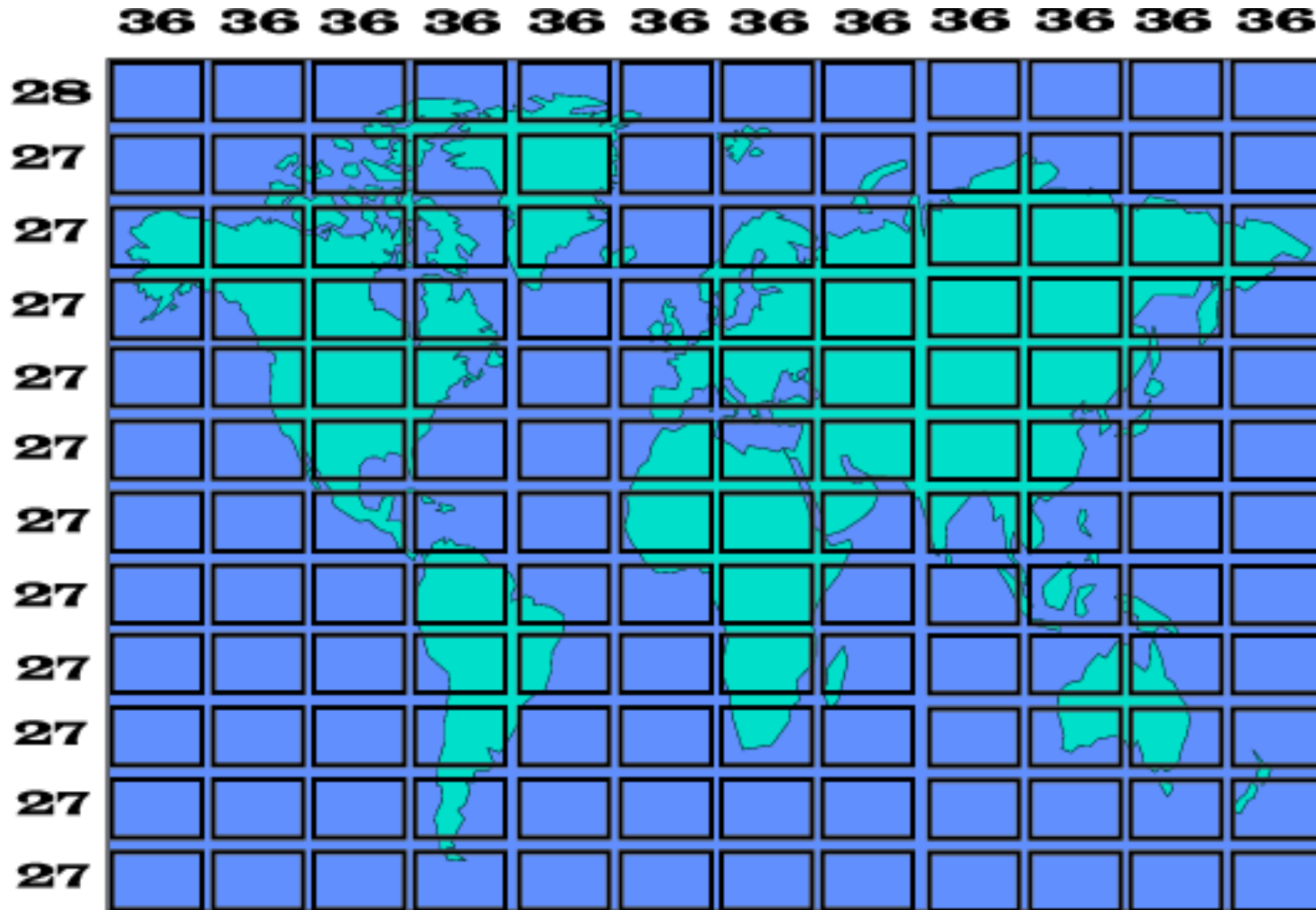
Optimisation for MPP

- ✓ Parallel read & packing of processed ensemble trajectory OK.
- ✓ Observation load imbalance (~50%) is not currently a major problem.
- Schur product routines are near top: need to use more processors.
- Horizontal domain decomposition is no longer sufficient with more processors: need to add time & ensemble-member.
- Possibly use OpenMP within nodes, with message-passing domain decomposition between nodes.

*Cost of a single 4DEnVar not a problem,
an ensemble of them might be.*



Horizontal domain decomposition:
144 pes for a 432x325 grid.





Optimisation - Algorithm

- Explore perturbation form of DEnKF: fewer iterations to solve for perturbations?
- Conjugate Gradient Algorithm with Hessian Eigenvector Preconditioning: existing software (Payne) & additional ideas (Desroziers & Berre 2012).
- Use Hessian eigenvectors directly to generate ensemble (EVIL, Auligné)



My understanding of EVIL

(following Tom Auligné)

4DEnVar grand transform \mathbf{U} :

$$\delta \mathbf{x} = \beta_c \mathbf{U}^c \mathbf{v}^c + \beta_e \sum_{m=1}^M \delta \mathbf{x}_m^f \circ (\mathbf{U}^e \mathbf{v}_m^e) = \mathbf{U} \mathbf{v}$$

Transformed Hessian

$$\frac{\partial^2 J}{\partial \mathbf{x}^2} = \mathbf{U}^{-T} \frac{\partial^2 J}{\partial \mathbf{v}^2} \mathbf{U}^{-1} = \mathbf{B}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} = \mathbf{A}^{-1}$$

Background and Analysis error covariances:

$$\mathbf{B} = \mathbf{U} \mathbf{U}^T, \quad \mathbf{A} = \mathbf{U} \left(\frac{\partial^2 J}{\partial \mathbf{v}^2} \right)^{-1} \mathbf{U}^T$$

Lanczos:

$$\left(\frac{\partial^2 J}{\partial \mathbf{v}^2} \right)^{-1} \approx \left(\mathbf{I} + \mathbf{Z}_K \left(\boldsymbol{\Theta}_K^{-\frac{1}{2}} - \mathbf{I} \right) \mathbf{Z}_K^T \right) \left(\mathbf{I} + \mathbf{Z}_K \left(\boldsymbol{\Theta}_K^{-\frac{1}{2}} - \mathbf{I} \right) \mathbf{Z}_K^T \right)^T$$

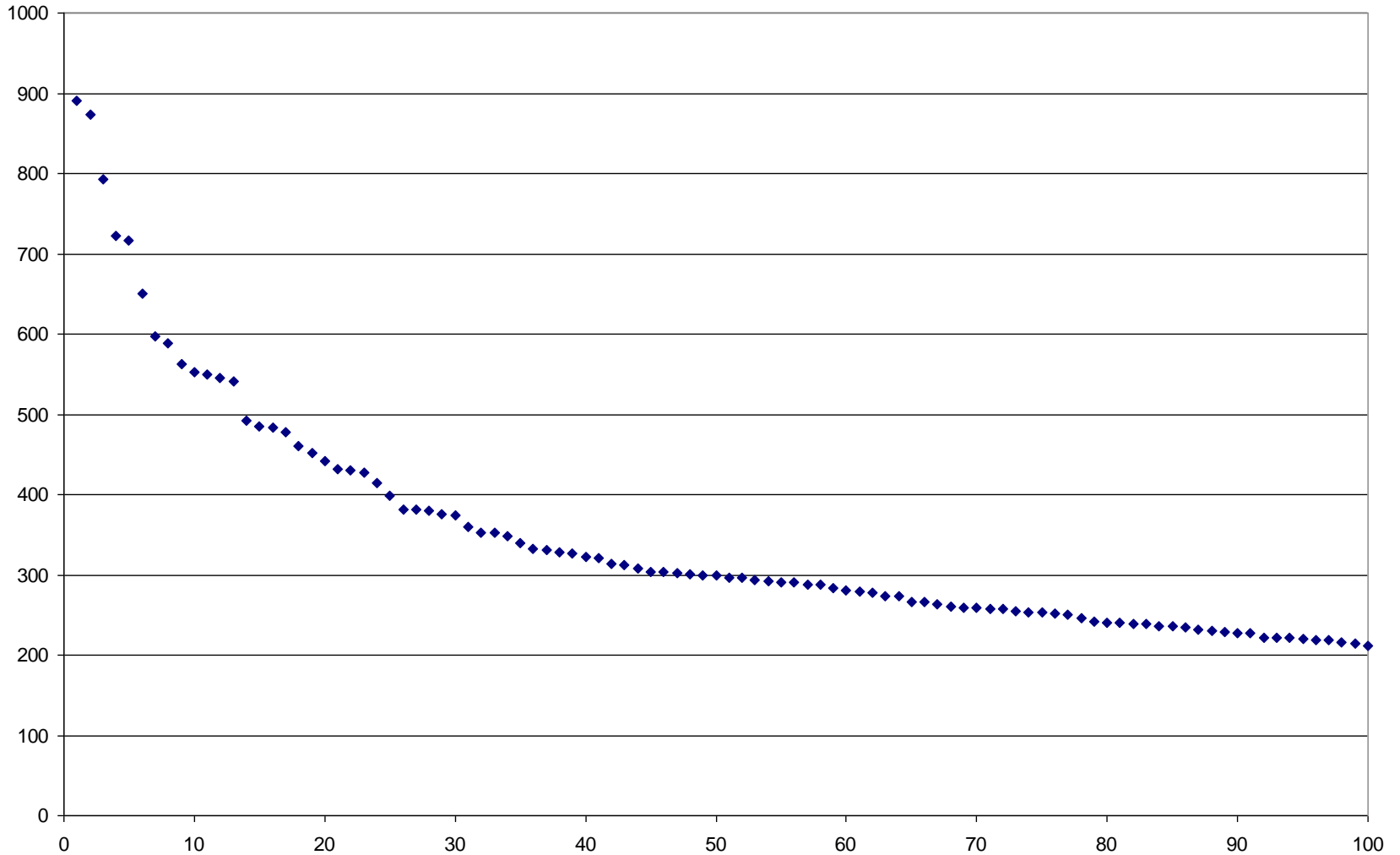
Find \mathbf{d}_m to recreate a forecast perturbation $\delta \mathbf{x}_m^f = \mathbf{U} \mathbf{d}_m$. Then

$$\delta \mathbf{x}_m^a = \mathbf{U} \left(\mathbf{I} + \mathbf{Z}_K \left(\boldsymbol{\Theta}_K^{-\frac{1}{2}} - \mathbf{I} \right) \mathbf{Z}_K^T \right) \mathbf{d}_m = \delta \mathbf{x}_m^f + \mathbf{U} \mathbf{Z}_K \left(\boldsymbol{\Theta}_K^{-\frac{1}{2}} - \mathbf{I} \right) \mathbf{Z}_K^T \mathbf{d}_m$$



Properties of Hessian

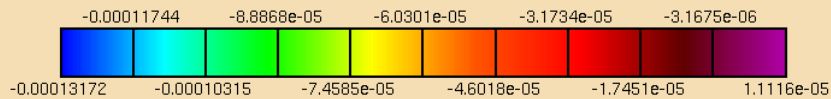
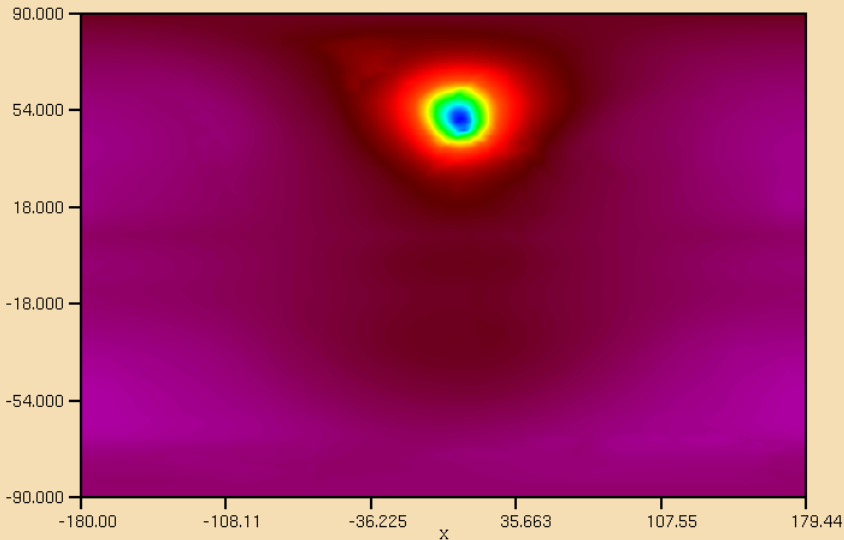
Hessian Eigenvalues from Global 3D-Var



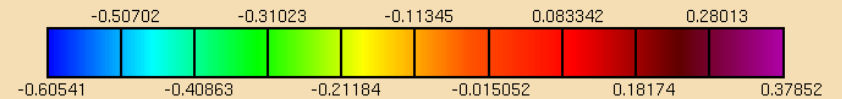
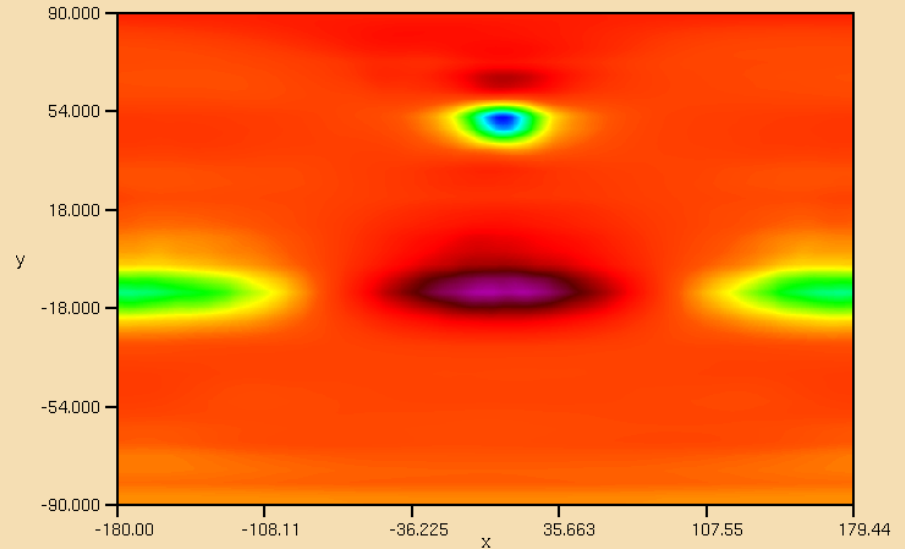


Typical Hessian eigenvectors

Unified Model Output (Vn 6.4): EXNER PRESSURE (RHO) AFTER TIMESTEP (Pa)
x: longitude (degrees_east)
y: latitude (degrees_north)
z: hybrid_ht 9.9977731704711914 (level)
t: date / t 2008/02/14:09.00 / 0.000000 (days since 2008-02-14 09:00:00)



Unified Model Output (Vn 6.4): THETA AFTER TIMESTEP (K)
x: longitude (degrees_east)
y: latitude (degrees_north)
z: hybrid_ht 51994.17578125 (level)
t: date / t 2008/02/14:09.00 / 0.000000 (days since 2008-02-14 09:00:00)





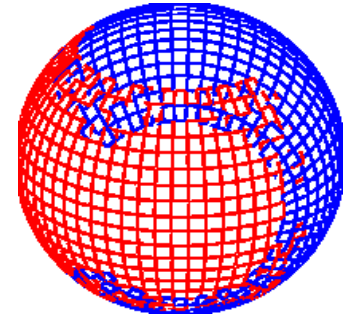
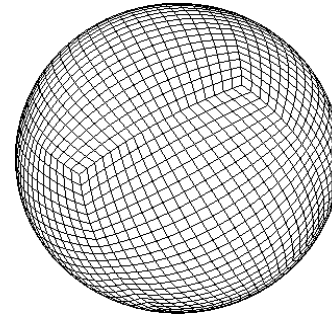
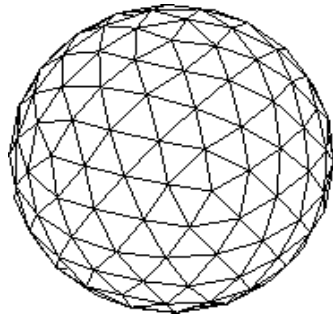
Development Plans

- **EnVar** (i.e. both hybrid-4D-Var & 4DEnVar)
 - Bigger ensemble. Tune hybrid β s.
 - Spectral localisation
 - Remove integrated divergence due to vertical localisation.
- **4DEnVar**
 - Tuning & optimisation
- **EDA** (i.e. an ensemble of 4DEnVar assimilations)
 - Inflation, perturbed obs or DEnKF, etc
 - Preconditioning or other efficient algorithm
 - Software optimisation (including ENDGAME model)



GungHo!

Globally
Uniform
Next
Generation
Highly
Optimized



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Met Office 4DEnVar system - Expectations

- **4DEnVar** is likely to be the **best strategy** on the timescale of GungHo: it is suitable for massively parallel computers and avoids writing the adjoint of the new model (decision 2015).
- We do not expect it to beat the current operational **hybrid-4D-Var** at same resolution, we are working to make it of comparable quality and cheaper.
- May be implemented to enable higher resolution forecasts, or frequent rapid runs to provide BCs for UK model.
- **Interesting** possibilities for **convective scale** and Nowcasting – need much **research!**
- An **ensemble of 4DEnVar** might beat operational local-ETKF. Several options for scientific & software design.

Nomenclature for Ensemble-Variational Data Assimilation

Recommendations by WMO's DAOS WG:

non-ambiguous terminology based on the most common established usage.

1. **En** should be used to abbreviate Ensemble, as in the EnKF.
2. No need for hyphens (except as established in 4D-Var)
3. **4D-Var** or **4DVAR** should only be used, even with a prefix, for methods using an adjoint model.
4. **EnVar** means a variational method using ensemble covariances. More specific prefixes (e.g. hybrid, 4D) may be added.
5. **hybrid** can be applied to methods using a combination of ensemble and climatological covariances.
6. The **EnKF** generate ensembles. **EnVar** does not, unless it is part of an ensemble of data assimilations (**EDA**).
7. **En4DVAR** could mean 4DVAR using ensemble covariances, but Liu et al. (2009) used it for something else. Less ambiguous is **4DVAR-Ben**.



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Questions and answers