Met Office

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

International Conference on Ensemble Methods in Geophysical Sciences, Toulouse, France, November 2012.

Andrew Lorenc, *Neill Bowler and Peter Jermey*

Outline of Talk

- Why are we doing it? What is wrong with 4D-Var? Addressed by:

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

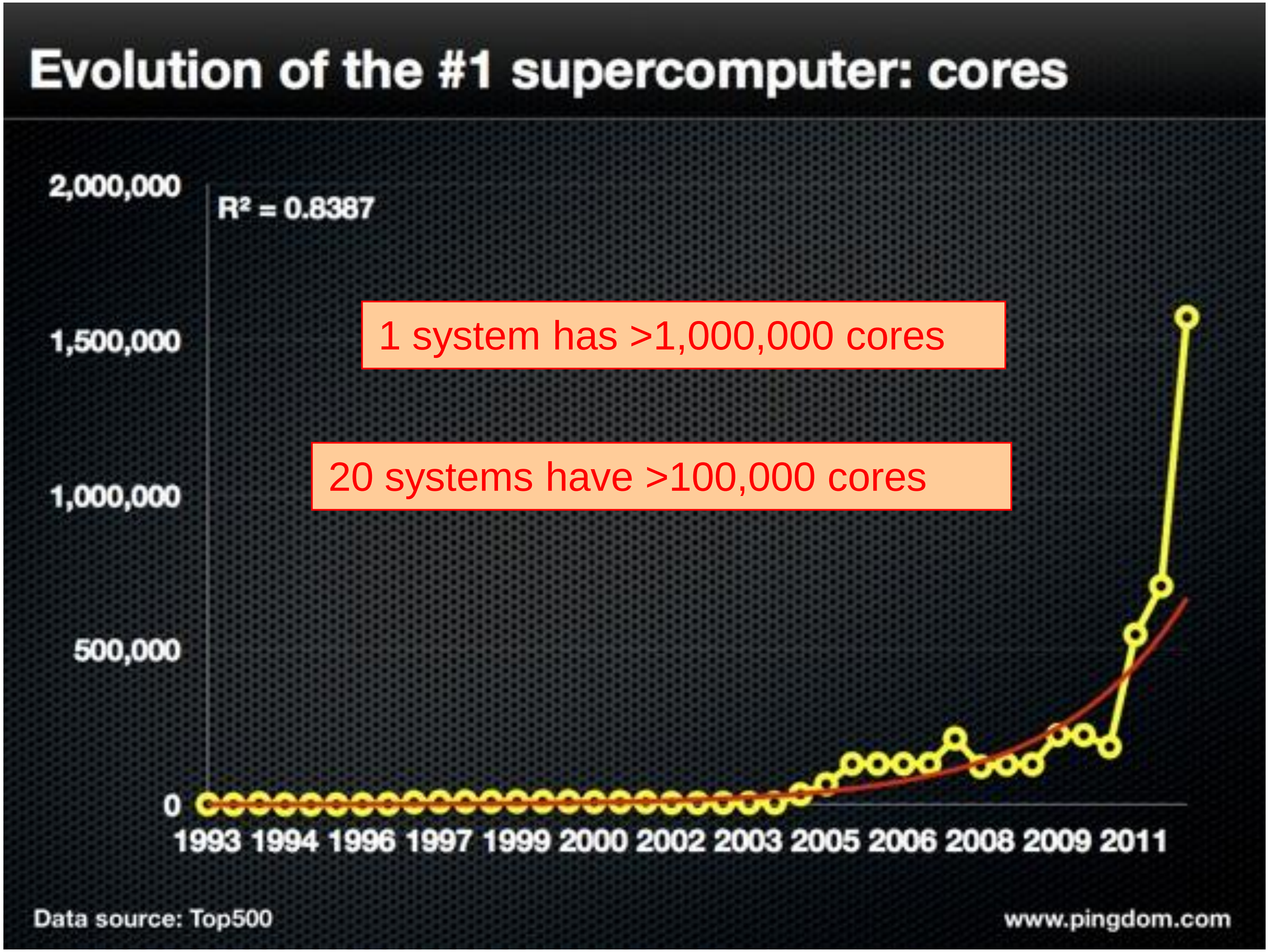
  4DEnVar. No need to integrate linear & adjoint models.

- Preliminary results of trials.
- Planned developments. What we expect to achieve.
- *Terminology (if time allows)*

Background

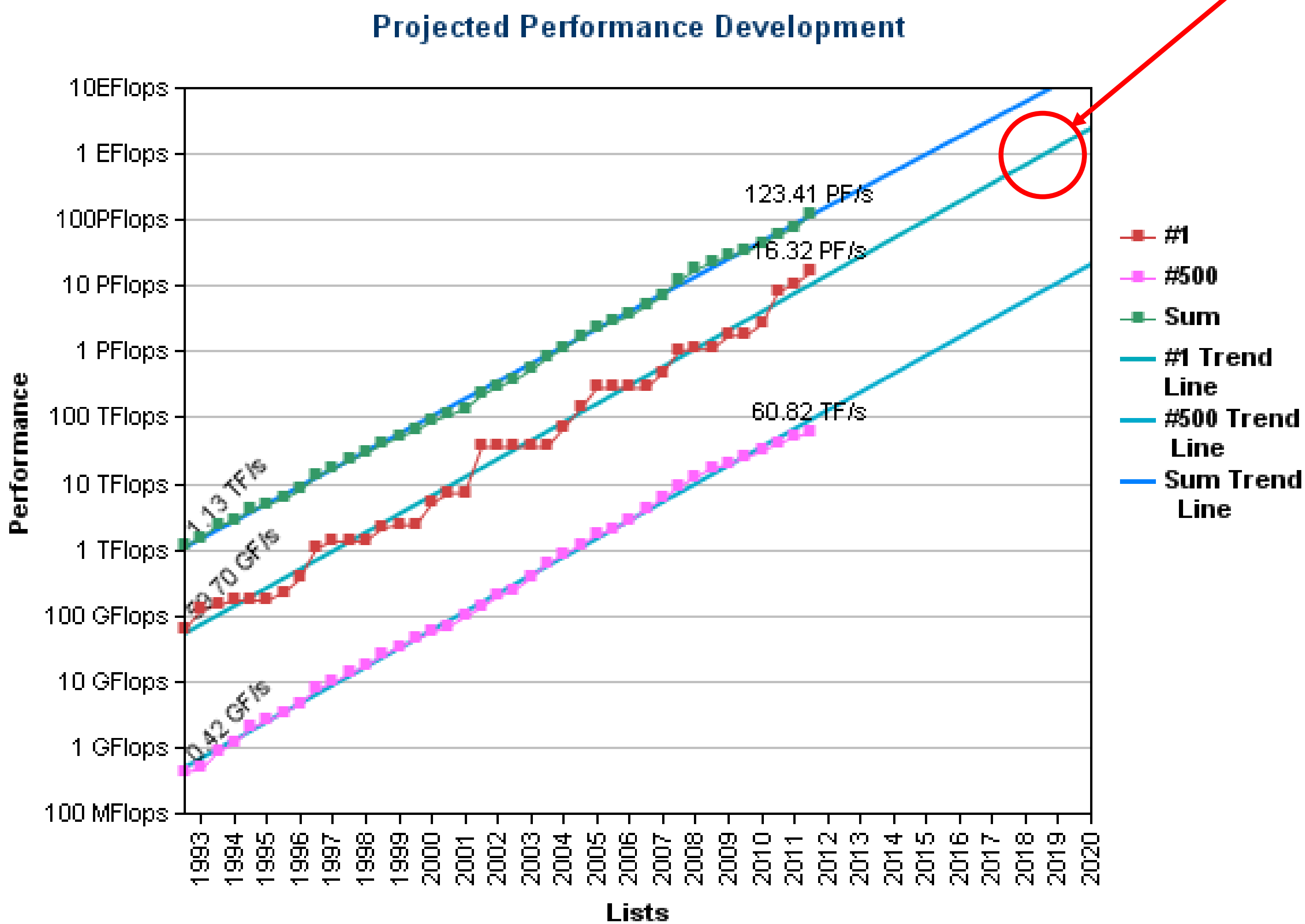
- 4D-Var has been the best DA method for operational NWP for the last decade (Rabier 2005).
- Since then we have gained a day's predictive skill – the forecast "background" is usually very good; properly identifying its likely errors is increasingly important.
- Most of the gain in skill has been due to increased resolution, which was enabled by bigger computers. To continue to improve, we must make effective use of planned massively parallel computers.

Top500 #1 Cores



Top500 projections

100M cores?



Nigel Wood

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 $\underline{M}$ and observation operator H

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

Measure misfit J of incremented state to background and observations

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

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

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

Key weaknesses of 4D-Var

1. Background errors are modelled using a covariance which is usually assumed to be stationary, isotropic and homogeneous.

2. The minimisation requires repeated sequential runs of a (low resolution) linear model and its adjoint.

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

This talk describes our 4DEnVar developments attempting to extend this to also address 2.

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

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

- Independent α_i implies that covariance of δx 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:

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

Hybrid 4D-Var formulation

Met Office

- 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 $\mathbf{P}_e \circ \mathbf{C}_{loc}$:

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

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

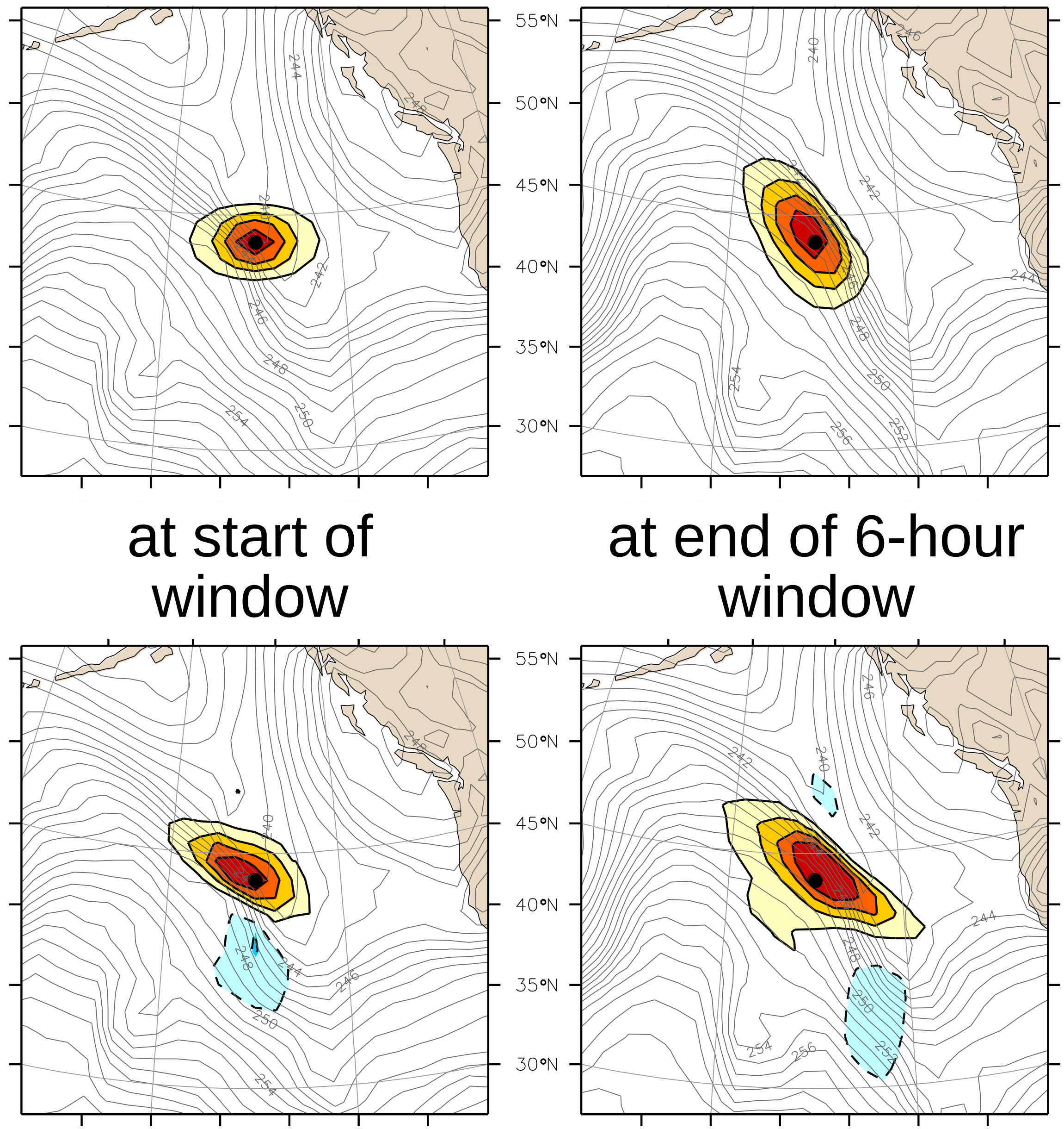
- Hybrid 4D-Var:

$$\mathbf{y} = H\left(\underline{M}\left(\mathbf{x}_b + \underline{\beta_c}\delta\mathbf{x}_c + \underline{\beta_e\delta\mathbf{x}_e}\right)\right)$$

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

- **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

Hybrid 4D-Var

Unfilled contours show T field.

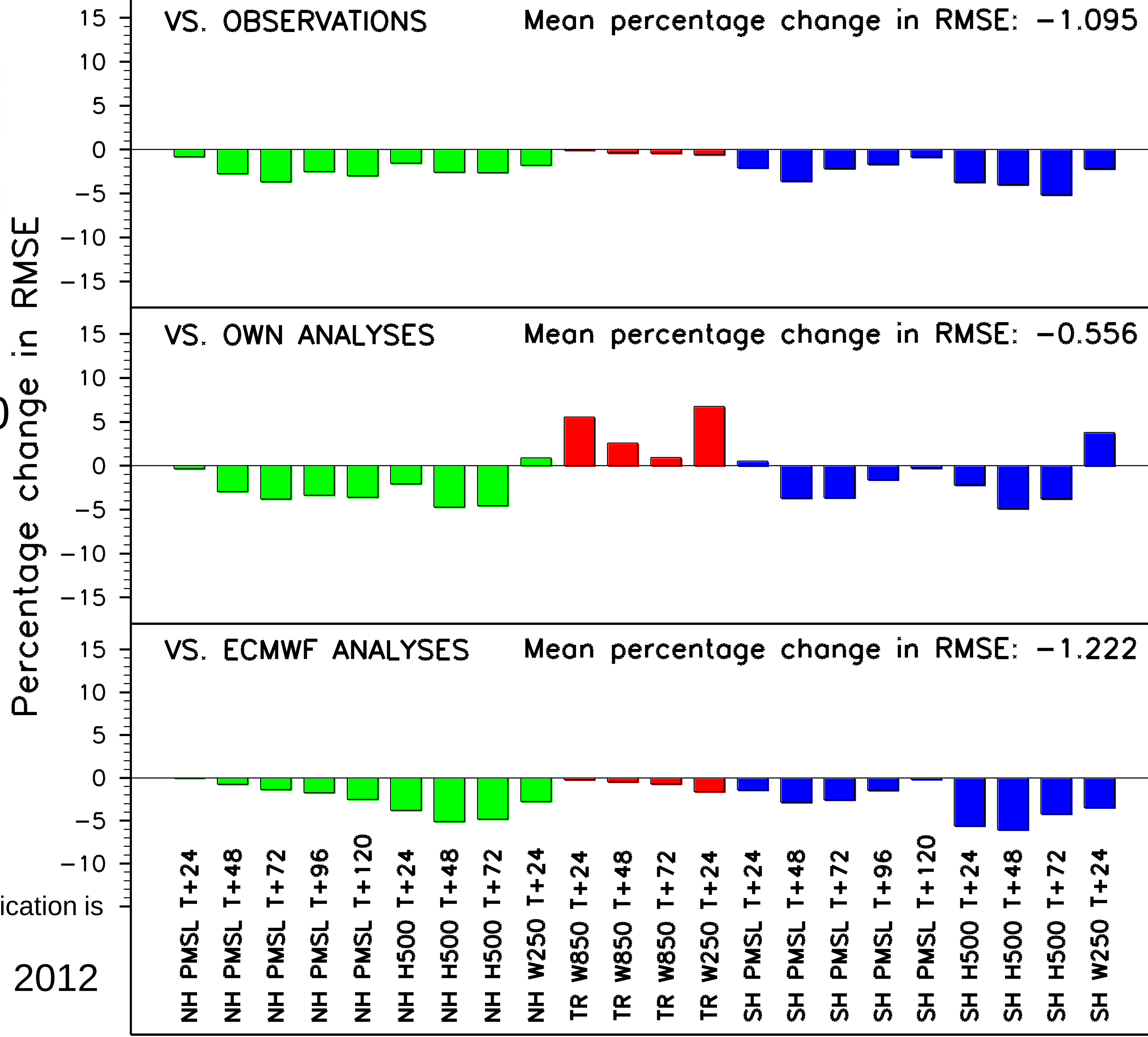
Clayton *et al.* 2012

Testing of hybrid 4D-Var

Met Office

- 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



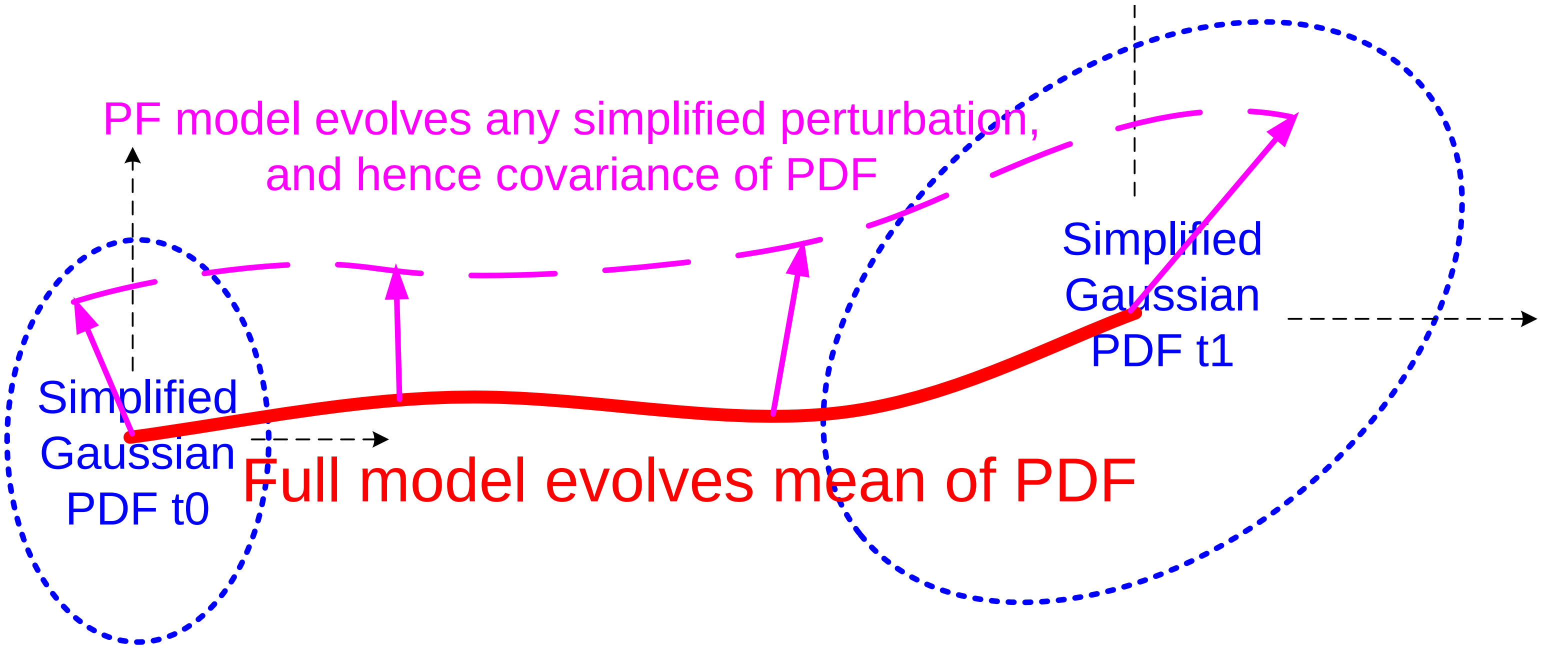
Own Analysis verification is unreliable.

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

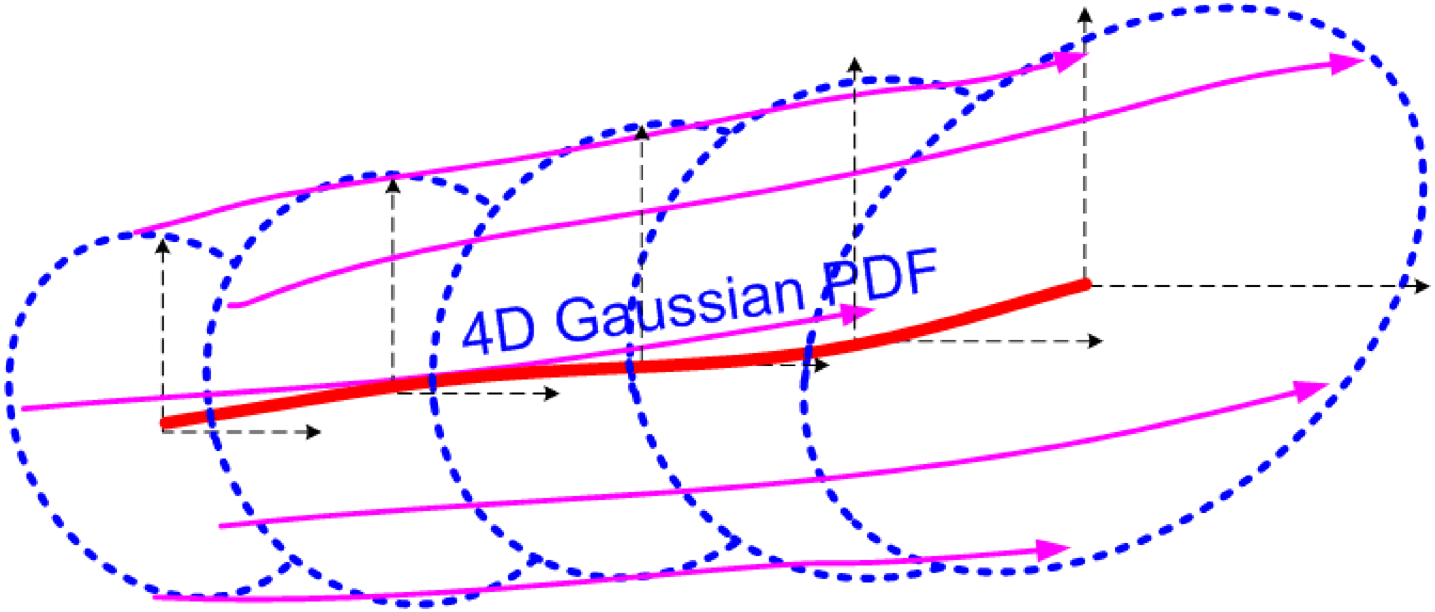


Statistical 4D-Var approximates entire PDF by a 4D Gaussian defined by PF model.

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

Lorenc & Payne 2007

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

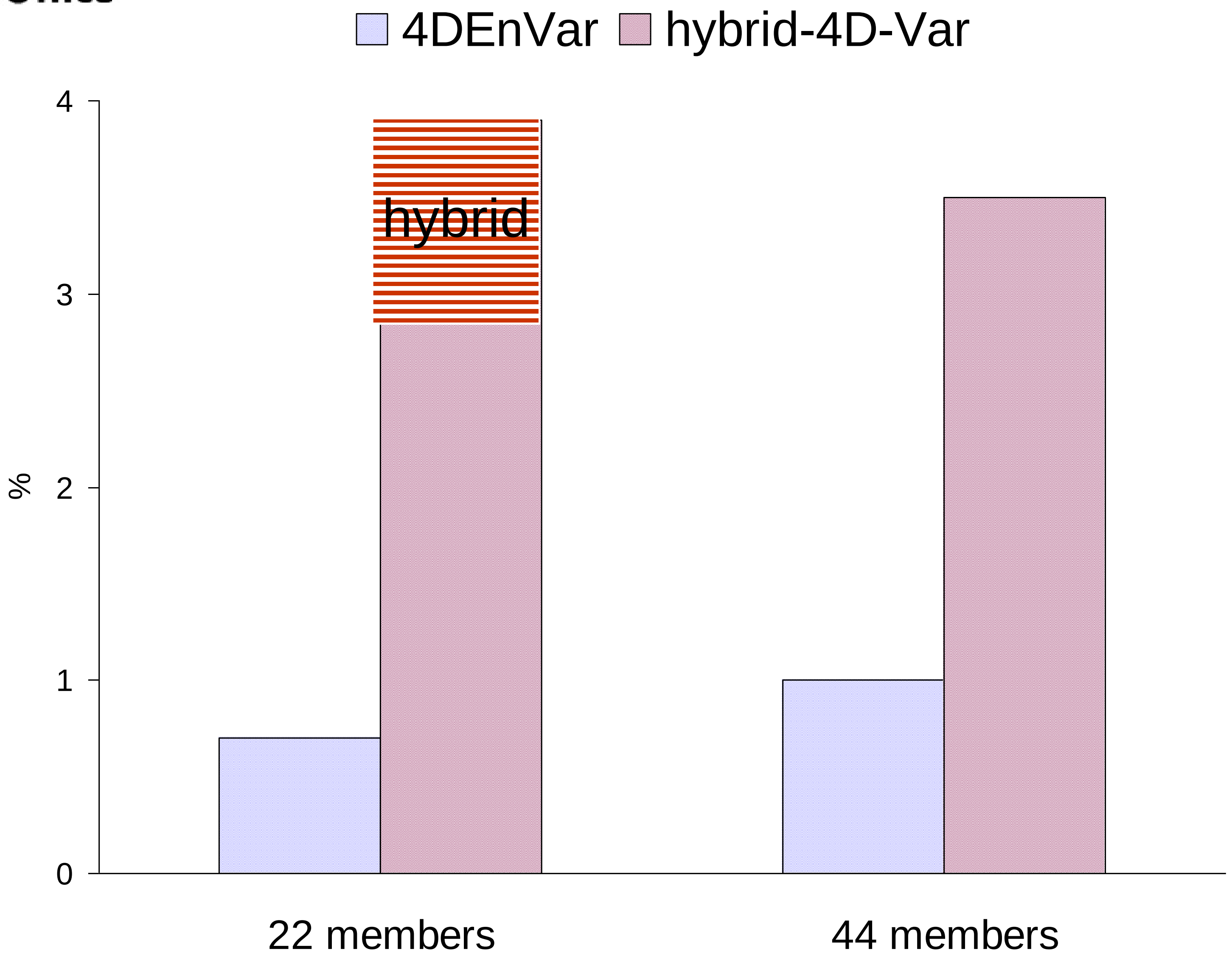
- 4D trajectory is used from background and ensemble, rather than 3D states at beginning of window.
- 4D localisation fields and increment $$\delta \underline{\mathbf{x}}_e = \frac{1}{\sqrt{K-1}} \sum_{i=1}^{K} (\underline{\mathbf{x}}_i - \overline{\underline{\mathbf{x}}}) \circ \underline{\boldsymbol{\alpha}}_i$$
- $\delta \underline{\mathbf{x}}_c$ 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.

Preliminary Results of Trials

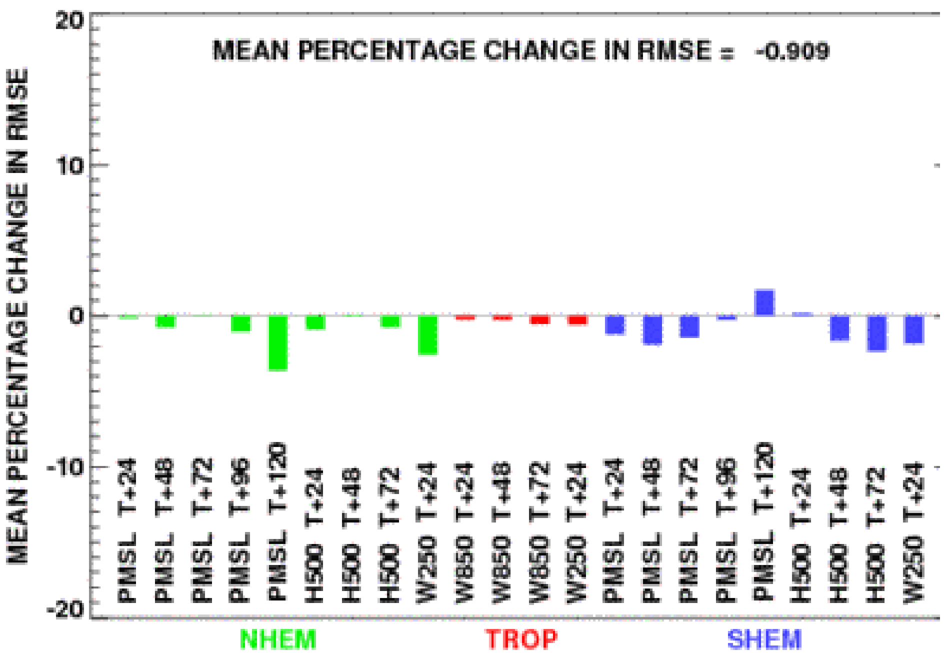
which are continuing …

- Target is to match operational hybrid-4D-Var
- 4DEnVar was set up with:
  - Same ensemble as hybrid-4D-Var
  - Same climatological **B** (but used as in **3**D-Var)
  - Same hybrid βs
  - 100 iterations
  - IAU-like initialisation
- Baseline is hybrid-3D-Var (≈3DEnVar)

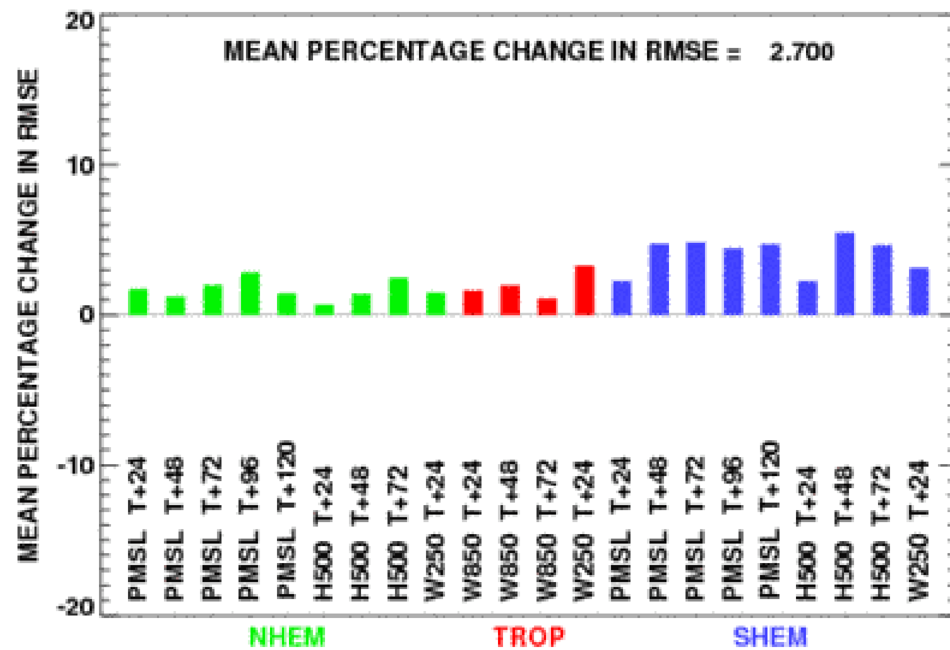
Mean RMS error reduction, compared to hybrid-3D-Var



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.

Preliminary timings

With 22 members, N216 resolution, 384 PEs on IBM P6

- Iterations in 4DEnVar were 11 times faster than in 4D-Var
- 30% of 4DEnVar in input & pre-processing of ensemble

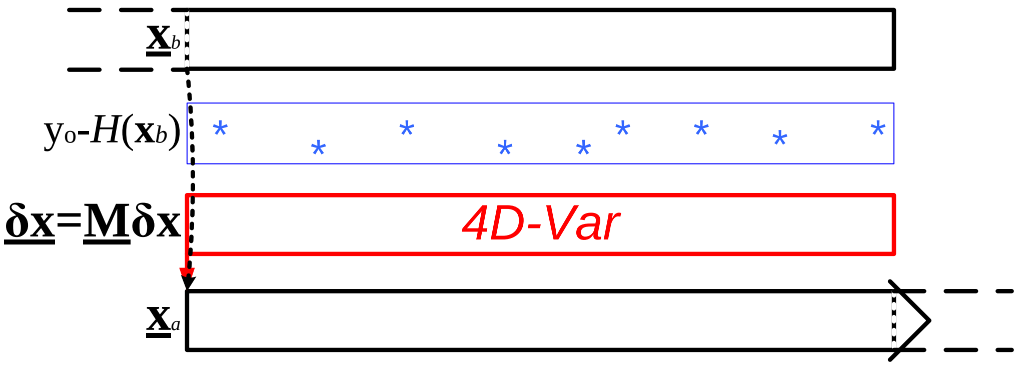
Complications in comparison

- Cost of ensemble forecasts not included
- 4DEnVar more scalable (no model solver)
- 4D-Var has a legacy of work to speed it up (multi−resolution, preconditioning)

Development Plans

- EnVar (i.e. both hybrid-4D-Var & 4DEnVar)
  - Bigger ensemble. Tune hybrid βs.
  - Spectral localisation (Buehner and Charron 2007)
  - Remove integrated divergence due to vertical localisation.
- 4DEnVar
  - Interface with forecast; Initialisation, e.g. IAU-like (Bloom *et al.* 1996)
  - Outer loop
- EDA (i.e. an ensemble of 4DEnVar assimilations)
  - Inflation, perturbed obs or DEnKF, etc (Bowler et al. 2012)
  - Preconditioning or other efficient algorithm (Desrozier & Berre 2012)

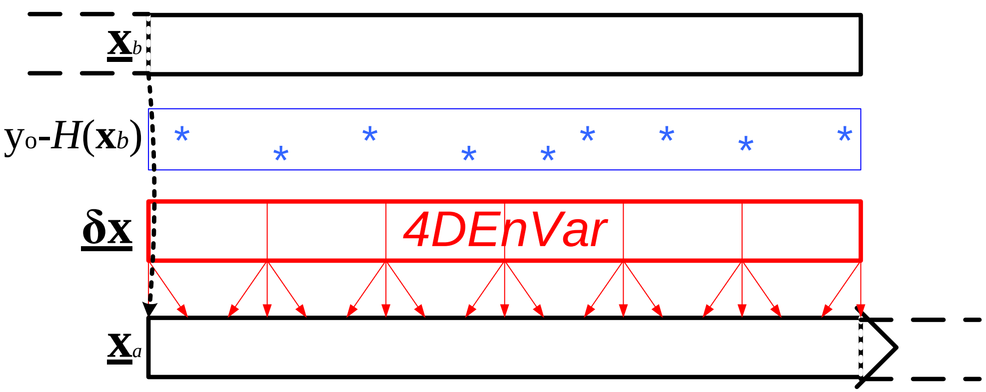
IAU-like interface with forecast model



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

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

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



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

There is no internal initialisation.

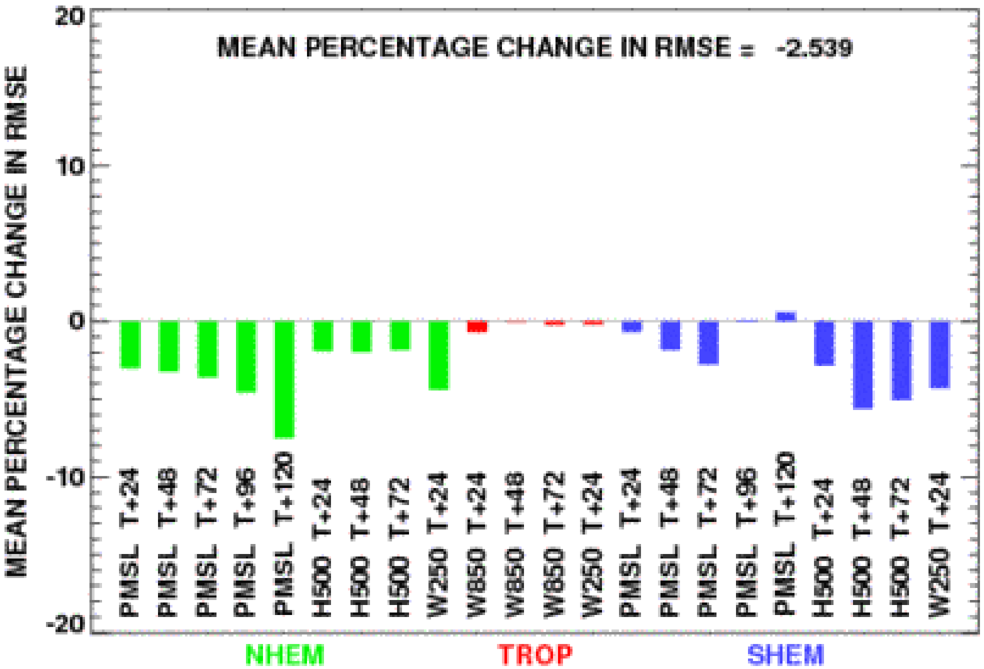
Nudge in $\underline{\boldsymbol{\delta}\mathbf{x}}$ during forecast, as part of an IAU-like initialisation.

Interface to forecast model has a very large impact on 4DEnVar.

4DEnVar with IAU-like interface

v

4DEnVar with 4D-Var-like interface



(22 member experiments.)

Met Office

GungHo!

Globally

Uniform

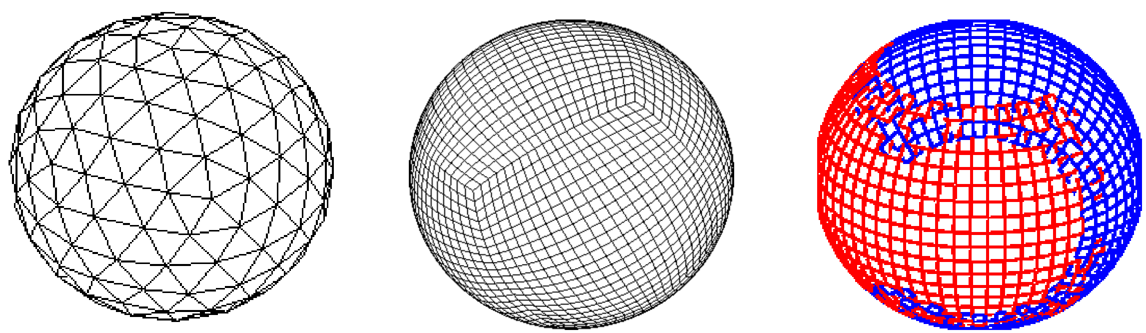
Next

Generation

Highly

Optimized

工合



NATURAL ENVIRONMENT RESEARCH COUNCIL

Science & Technology Facilities Council

"Working together harmoniously"

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 (talk by Stephen Pring later); 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.

References

Bloom SC, Takacs LL, Silva AMD, Ledvina D. 1996. Data assimilation using incremental analysis updates. *Mon. Weather Rev.* **124**: 1256–1271.

Bowler NE, Flowerdew J, Pring SR. 2012. Tests of different flavours of EnKF on a simple model. *Q. J. R. Meteorol. Soc.* **accepted**: 14pp.

Buehner M, Charron M. 2007. Spectral and spatial localization of background-error correlations for data assimilation. *Q. J. R. Meteorol. Soc.* **133**(624): 615–630.

Buehner M, Houtekamer PL, Charette C, Mitchell HL, He B. 2010a. Intercomparison of variational data assimilation and the ensemble Kalman filter for global deterministic NWP. part i: Description and single-observation experiments. *Mon. Weather Rev.* **138**: 1550–1566.

Buehner M, Houtekamer PL, Charette C, Mitchell HL, He B. 2010b. Intercomparison of variational data assimilation and the ensemble Kalman filter for global deterministic NWP. part ii: One-month experiments with real observations. *Mon. Weather Rev.* **138**: 1567–1586.

Clayton AM, Lorenc AC, Barker DM. 2012. Operational implementation of a hybrid ensemble/4D-Var global data assimilation system at the Met Office. *Q. J. R. Meteorol. Soc.* **accepted**: 16pp.

Desroziers G, Berre L. 2012. Accelerating and parallelizing minimizations in ensemble and deterministic variational assimilations. *Q. J. R. Meteorol. Soc.* **138**(667): 1599–1610.

Hunt B, Kalnay E, Kostelich E, Ott E, Patil D, Sauer T, Szunyogh I, Yorke J, Zimin A. 2004. Four-dimensional ensemble Kalman filtering. *Tellus A* **56**(4): 273–277.

Liu C, Xiao Q, Wang B. 2008. An ensemble-based four-dimensional variational data assimilation scheme. part i: Technical formulation and preliminary test. *Mon. Weather Rev.* **136**: 3363–3373.

Liu C, Xiao Q, Wang B. 2009. An ensemble-based four-dimensional variational data assimilation scheme. part ii: Observing System Simulation Experiments with advanced research WRF (ARW). *Mon. Weather Rev.* **137**: 1687–1704.

Lorenc AC. 2003. The potential of the ensemble Kalman filter for NWP - a comparison with 4D-Var. *Q. J. R. Meteorol. Soc.* **129**: 3183–3203.

Lorenc AC, Payne T. 2007. 4D-Var and the butterfly effect: Statistical four-dimensional data assimilation for a wide range of scales. *Q. J. R. Meteorol. Soc.* **133**: 607–614.

Rabier F. 2005. Overview of global data assimilation developments in numerical weather-prediction centres. *Q. J. R. Meteorol. Soc.* **131**(613): 3215–3233.

Wang X, Barker DM, Snyder C, Hamill TM. 2008a. A hybrid ETKF-3DVAR data assimilation scheme for the wrf model. part i: Observing system simulation experiment. *Mon. Weather Rev.* **136**: 5116–5131.

Wang X, Barker DM, Snyder C, Hamill TM. 2008b. A hybrid ETKF-3DVAR data assimilation scheme for the WRF model. part ii: Real observation experiments. *Mon. Weather Rev.* **136**: 5132–5147.

Wang X, Snyder C, Hamill TM. 2007. On the theoretical equivalence of differently proposed ensemble–3DVAR hybrid analysis schemes. *Mon. Weather Rev.* **135**(1): 222–227.

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**.