Four-Dimensional Ensemble-Variational Data Assimilation 4DEnVar

Colloque National sur l'Assimilation de données

Andrew Lorenc, **Toulouse France. 1-3 décembre 2014**

4DEnVar: Topics in Talk

- Design
- Comparison with 4DVar
- Localisation & filtering of ensemble covariance
- Plans

Data Assimilation for Numerical Weather Prediction
Design of a Modern System

Bayesian combination of observations and prior (background)

Incremental formulation – find best correction to prior

Cycled DA – each cycle assimilates a batch of observations spread over a time-window

Gaussian assumptions about Probability Distribution Functions

"Errors Of The Day" information in prior (background) PDF comes from an ensemble of forecasts.

Four-Dimensional Variational DA Methods

Ours are **incremental**, with **no outer-loop** and **no model error terms**.

Each gives a 4D best-fit to prior & observations in a 6 hour window.

Use underline to denote 4D variables and operators:

$\underline{\mathbf{x}}^b$	background trajectory
$\underline{\mathbf{P}}$	4D error covariance of $\underline{\mathbf{x}}^b$
$\delta\underline{\mathbf{x}}$	4D analysis increment
$\underline{\mathbf{y}} = \underline{H}\left(\underline{\mathbf{x}}^b + \delta\underline{\mathbf{x}}\right)$	model estimate of obs
$J\left(\delta\underline{\mathbf{x}}\right) = \frac{1}{2}\delta\underline{\mathbf{x}}^T\underline{\mathbf{P}}^{-1}\delta\underline{\mathbf{x}} + \frac{1}{2}\left(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o\right)^T\underline{\mathbf{R}}^{-1}\left(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o\right)$	penalty function

4DVar uses linear model $\delta\underline{\mathbf{x}} = \underline{\mathbf{M}}\delta\mathbf{x}_0$

4DEnVar uses a linear combination of perturbation trajectories $\delta\underline{\mathbf{x}} = \Sigma_{k=1}^{N}\underline{\boldsymbol{\alpha}}_k \circ \underline{\mathbf{x}}'_k$

hybrid $\Rightarrow$ a combination of climatological and localized ensemble covariances.

Possible Methods

- **[Hybrid / Ensemble] - 4DVar**
  Use ensemble to augment 3D covariance at beginning of window, then use linear & adjoint model for time-dimension.

- **[Hybrid] - 4DEnVar**
  Use ensemble trajectories to determine 4D covariance directly.

- **EnKF – e.g. 4D-LETKF**
  Localised Ensemble Transform Kalman Filter – transforms background ensemble perturbations to sample the analysed PDF from Kalman eqn.

All need to use [localisation / smoothing / hybridisation] to get usable covariances from a small ensemble!!

Met Office

4DEnVar: using an ensemble of 4D trajectories which samples background errors

Ensemble trajectory matrix $\underline{\mathbf{X}} = \left[\underline{\mathbf{x}}'_1 \ \cdots \ \underline{\mathbf{x}}'_N \right]$ where $\underline{\mathbf{x}}'_k = \frac{1}{\sqrt{N-1}} \left(\underline{\mathbf{x}}_k - \bar{\underline{\mathbf{x}}} \right)$

Model 4D $\underline{\mathbf{P}}$ directly, as localised ensemble covariance,

$$\underline{\mathbf{P}} = \underline{\mathbf{C}} \circ \underline{\mathbf{X}}\underline{\mathbf{X}}^T$$

then model $\underline{\mathbf{C}}$ using transforms

$$\underline{\mathbf{C}} = \underline{\mathbf{U}}^\alpha \underline{\mathbf{U}}^{\alpha T}$$

4D localised linear combination of ensemble trajectories

$$\underline{\boldsymbol{\alpha}}_k = \underline{\mathbf{U}}^\alpha \mathbf{v}_k^\alpha$$

$$\delta\underline{\mathbf{x}} = \Sigma_{k=1}^{N} \underline{\boldsymbol{\alpha}}_k \circ \underline{\mathbf{x}}'_k$$

concatenated control vectors

$$\mathbf{v}^T = \left[\mathbf{v}_1^{\alpha T} \cdots \mathbf{v}_N^{\alpha T} \right]$$

Transformed penalty function

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

4DEnVar: using an ensemble of 4D trajectories which samples background errors

Extra Details

model $\underline{\mathbf{C}}$ using transforms

$$\underline{\mathbf{C}} = \underline{\mathbf{U}}^{\alpha}\underline{\mathbf{U}}^{\alpha T}$$

It is common to use a 3D $\mathbf{C}$

$$\mathbf{C} = \mathbf{U}^{\alpha}\mathbf{U}^{\alpha T}$$

and persistence in time: $\underline{\mathbf{I}}$

$$\underline{\mathbf{C}} = \underline{\mathbf{I}}\mathbf{C}\underline{\mathbf{I}}^{T}$$

4D localised linear combination of ensemble trajectories

$$\delta\underline{\mathbf{x}} = \sum_{k=1}^{N} \underline{\boldsymbol{\alpha}}_k \circ \underline{\mathbf{x}}'_k$$

can be built from 3D localised perturbations and constant $\boldsymbol{\alpha}_k$.

$$\boldsymbol{\alpha}_k = \mathbf{U}^{\alpha}\mathbf{v}_k^{\alpha}$$

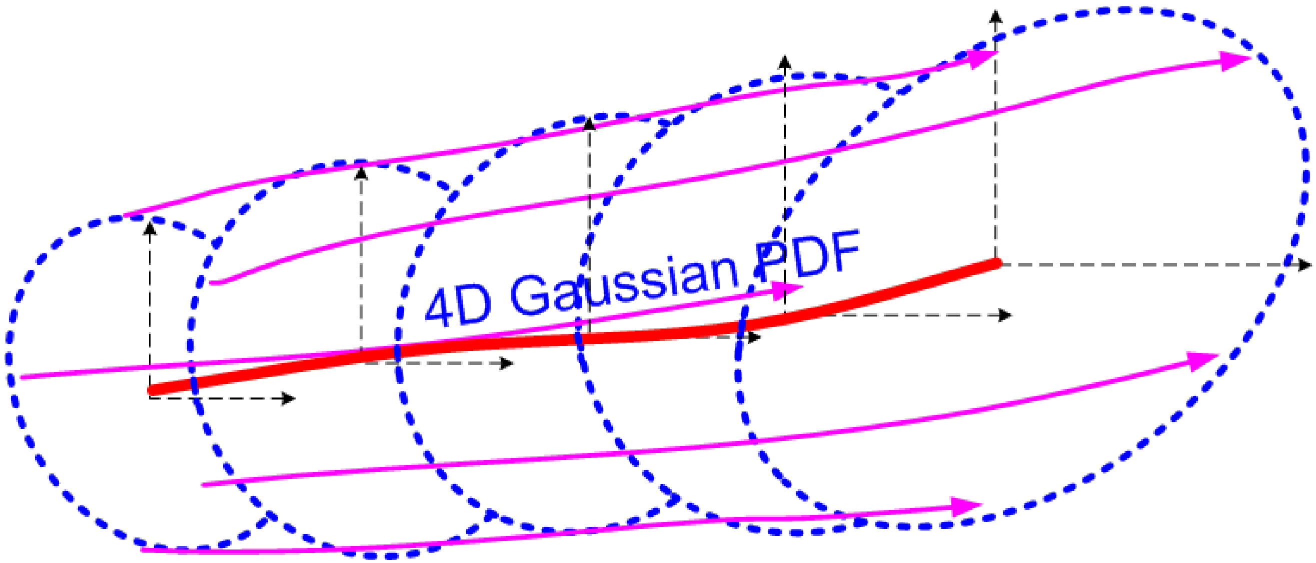
$$\delta\mathbf{x}\left(t\right) = \sum_{k=1}^{N} \boldsymbol{\alpha}_k \circ \mathbf{x}'_k\left(t\right)$$

Matrix notation:

Buehner (2005) avoids $\circ$ using $diag\left(\mathbf{x}\right)$ for the diagonal matrix: $diag\left(\mathbf{x}\right)_{i,i} = \mathbf{x}_i$

$$\delta\mathbf{x}\left(t\right) = \sum_{k=1}^{N} diag\left(\mathbf{x}'_k\left(t\right)\right)\boldsymbol{\alpha}_k$$

Incremental 4D-Ensemble-Var



Trajectories of perturbations from ensemble mean

Ensemble mean trajectory

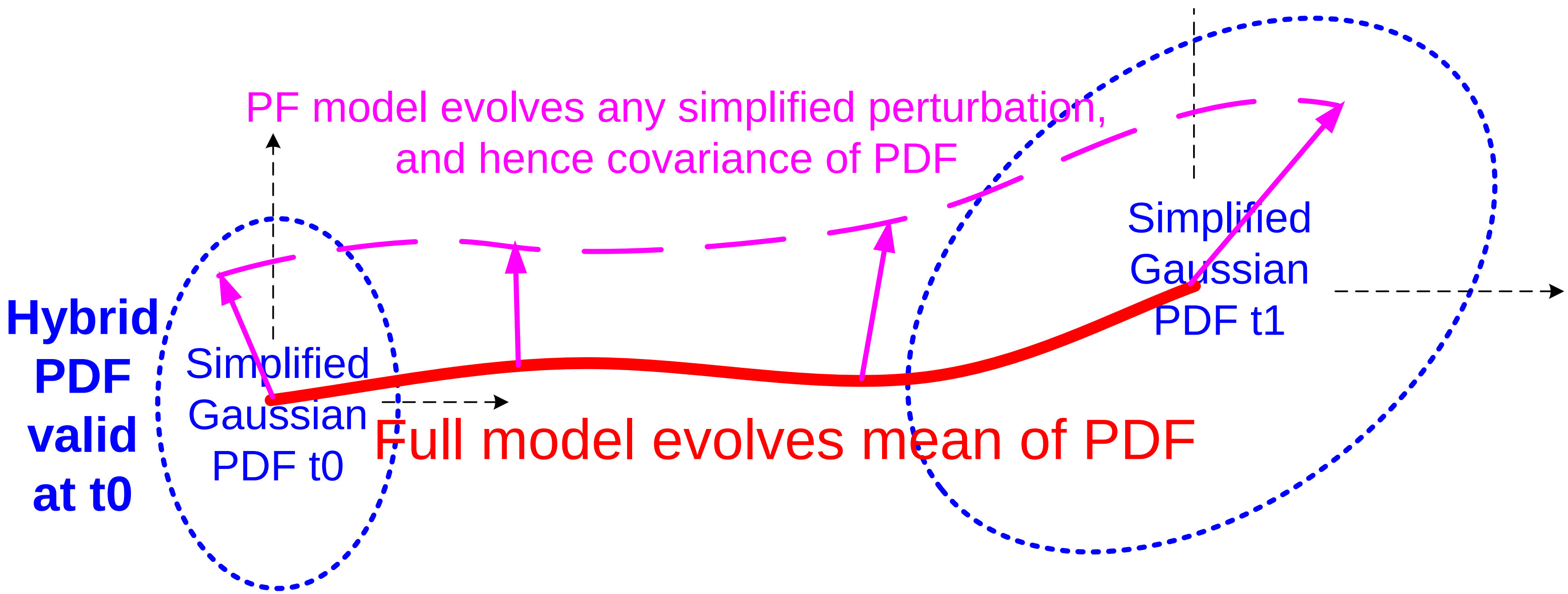
Localised trajectories define 4D PDF of possible increments

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

4D analysis is a (localised) linear combination of nonlinear trajectories. It is not itself a trajectory.

Comparison with 4DVar

Statistical, incremental 4DVar



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

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

Lorenc & Payne 2007

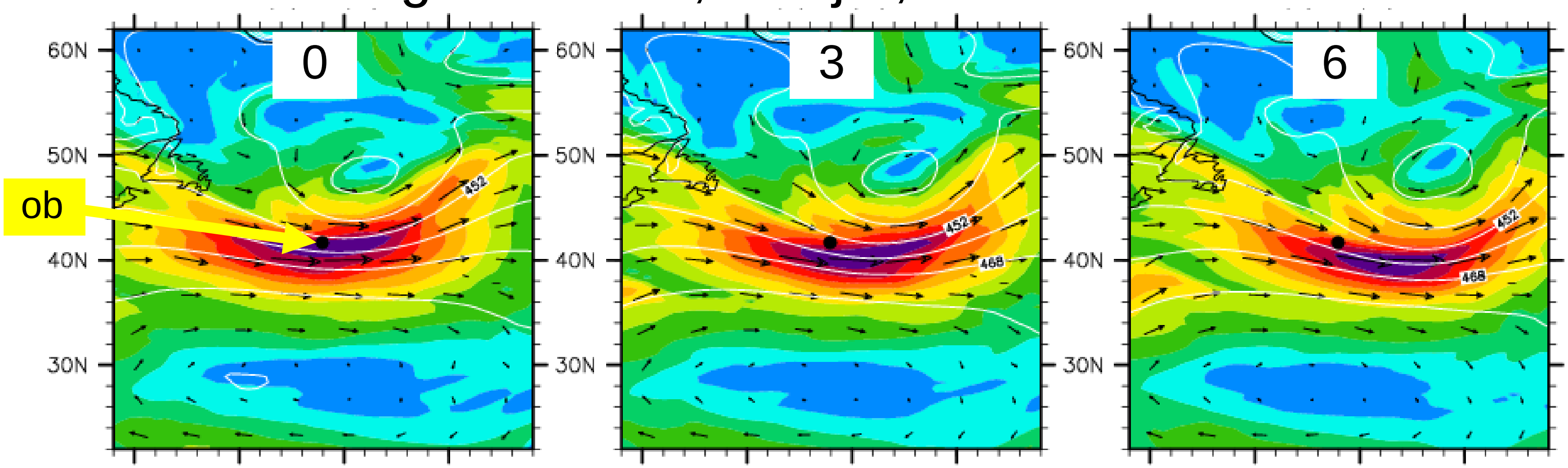
A new form of linear model

Met Office

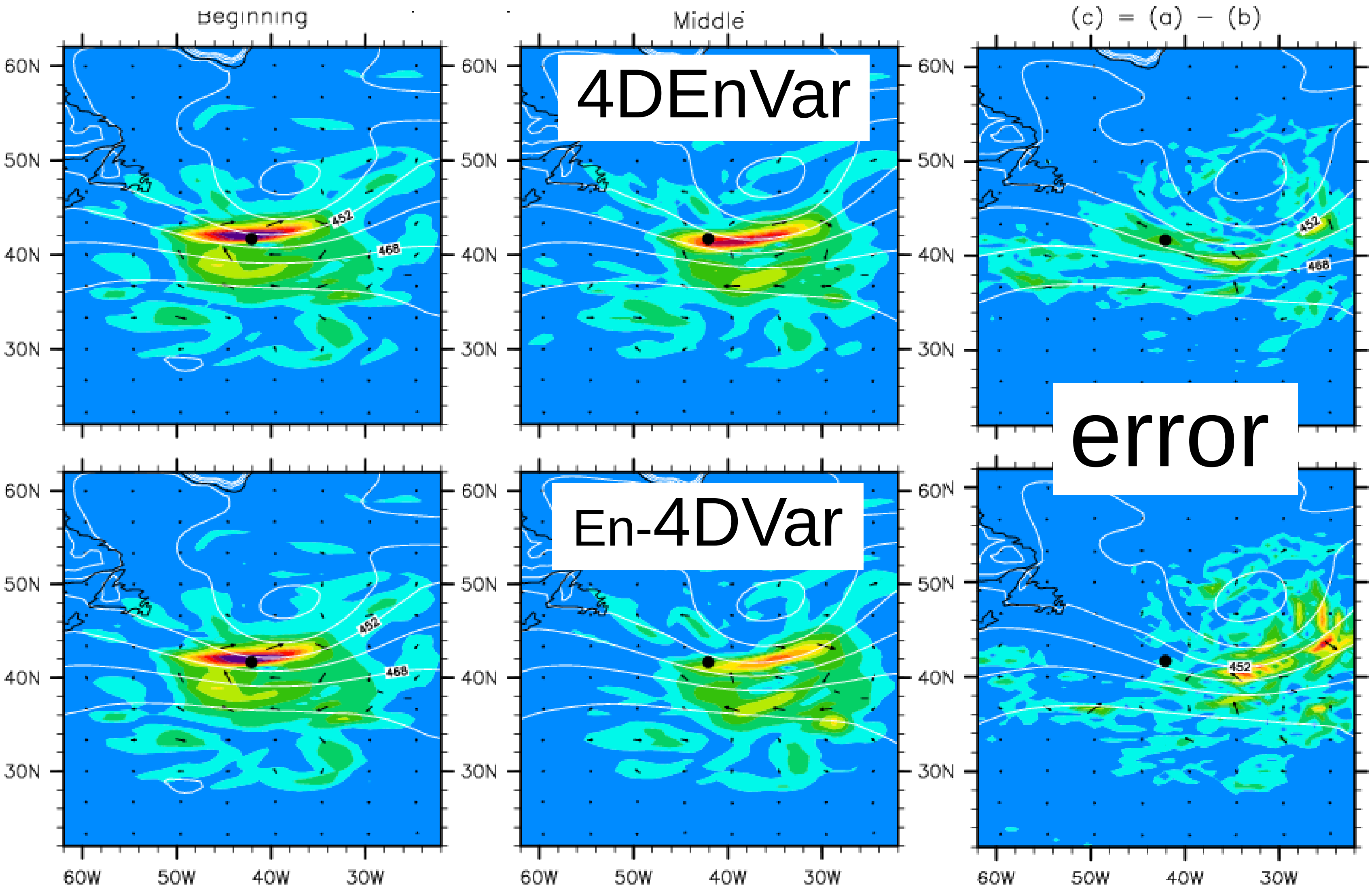
En-4DVar analysis increment $\delta\underline{\mathbf{x}} = \underline{\mathbf{M}}\, \Sigma_{k=1}^{N} \boldsymbol{\alpha}_k \circ \mathbf{x}'_k$

4DEnVar analysis increment $\delta\underline{\mathbf{x}} = \Sigma_{k=1}^{N} \underline{\boldsymbol{\alpha}}_k \circ \underline{\mathbf{x}}'_k$

Test with a single wind ob, in a jet, at the start of the window



100% ensemble
1200km localization scale



hybrid-4DEnVar

4D analysis increment $\delta\underline{\mathbf{x}} = \beta_c \underline{\mathbf{I}}\delta\mathbf{x}_0 + \beta_e \Sigma_{k=1}^{N} \underline{\boldsymbol{\alpha}}_k \circ \underline{\mathbf{x}}'_k$

Localized 4D covariance $\underline{\mathbf{P}} = \beta_c^2 \underline{\mathbf{I}}\mathbf{B}\underline{\mathbf{I}}^T + \beta_e^2 \underline{\mathbf{C}} \circ \underline{\mathbf{X}}\underline{\mathbf{X}}^T$

hybrid-4DVar

4D analysis increment $\delta\underline{\mathbf{x}} = \underline{\mathbf{M}}\left(\beta_c \delta\mathbf{x}_0 + \beta_e \Sigma_{k=1}^{N} \boldsymbol{\alpha}_k \circ \mathbf{x}'_k\right)$

Localized 4D covariance $\underline{\mathbf{P}} = \underline{\mathbf{M}}\left(\beta_c^2 \mathbf{B} + \beta_e^2 \mathbf{C} \circ \mathbf{X}\mathbf{X}^T\right)\underline{\mathbf{M}}^T$

Met Office trial of 4DEnVar

Lorenc et al. (2014)

Our first trial copied settings from the hybrid-4DVar:

- C with localisation scale 1200km,
- hybrid weights β_c^2=0.8, β_e^2=0.5

Results were disappointing:

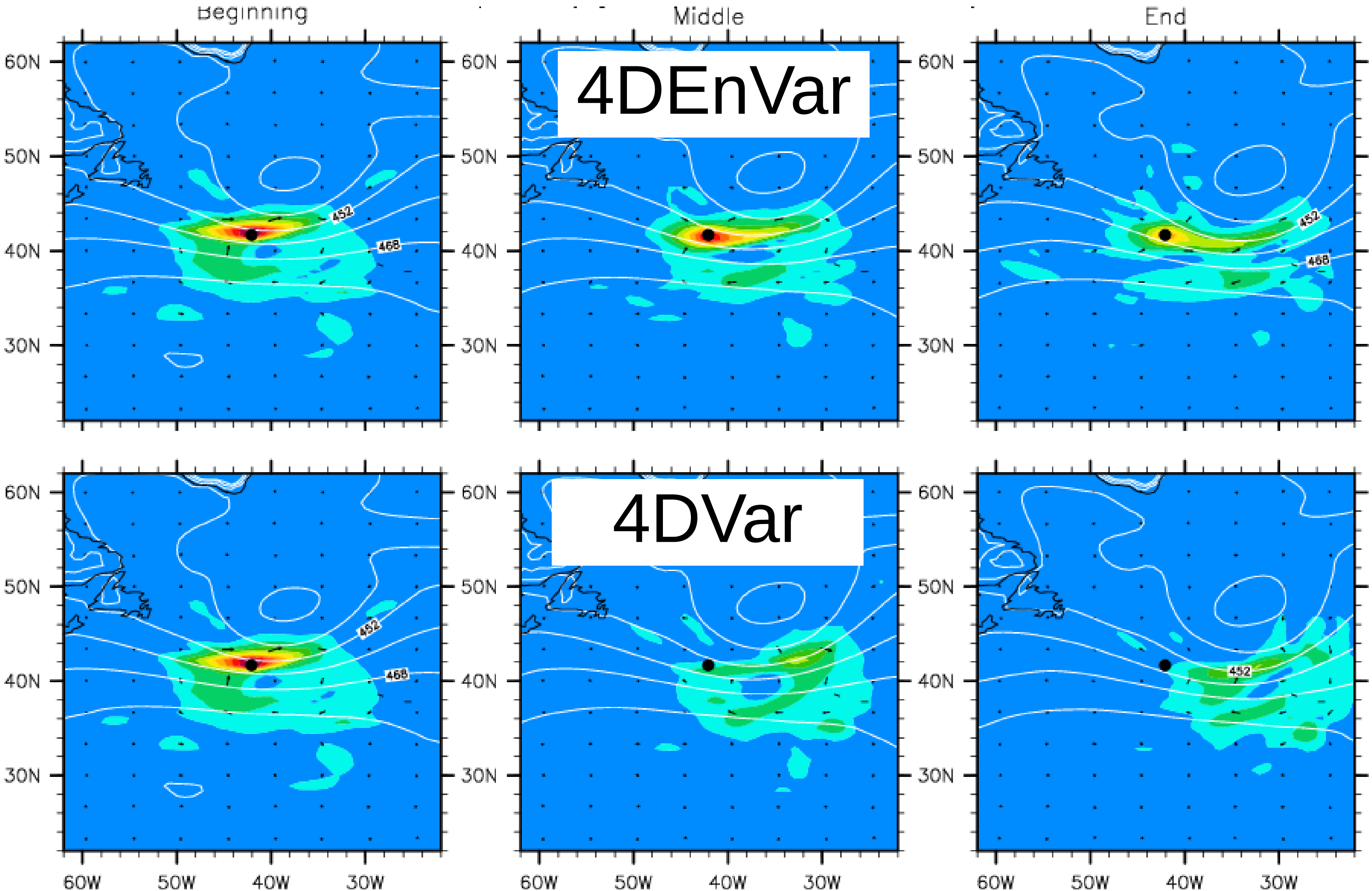
hybrid-4DVar
3.6% better

hybrid-4DEnVar
0.5% better

hybrid-3DVar = hybrid-3DEnVar

The reason was the large weight given to the climatological covariance, which is treated like 3DVar in 4DEnVar

50-50% hybrid
1200km localization scale



Relative "Strong Constraint Errors"

Met Office

We ran similar tests on a Hurricane Sandy case.
Here the ensemble covariances dominated, making hybrid-4DEnVar perform better.

1200km localization scale	Jet case	Hurricane Sandy
4DEnVar	51%	57%
En-4DVar	54%	69%
Hybrid-4DEnVar	78%	66%
Hybrid-4DVar	66%	75%

When the ensemble covariances dominated the increments,
and the horizontal localisation was not too severe,
4DEnVar had better consistency with the strong constraint than 4DVar.

Runs with smallest deviation from model constraint

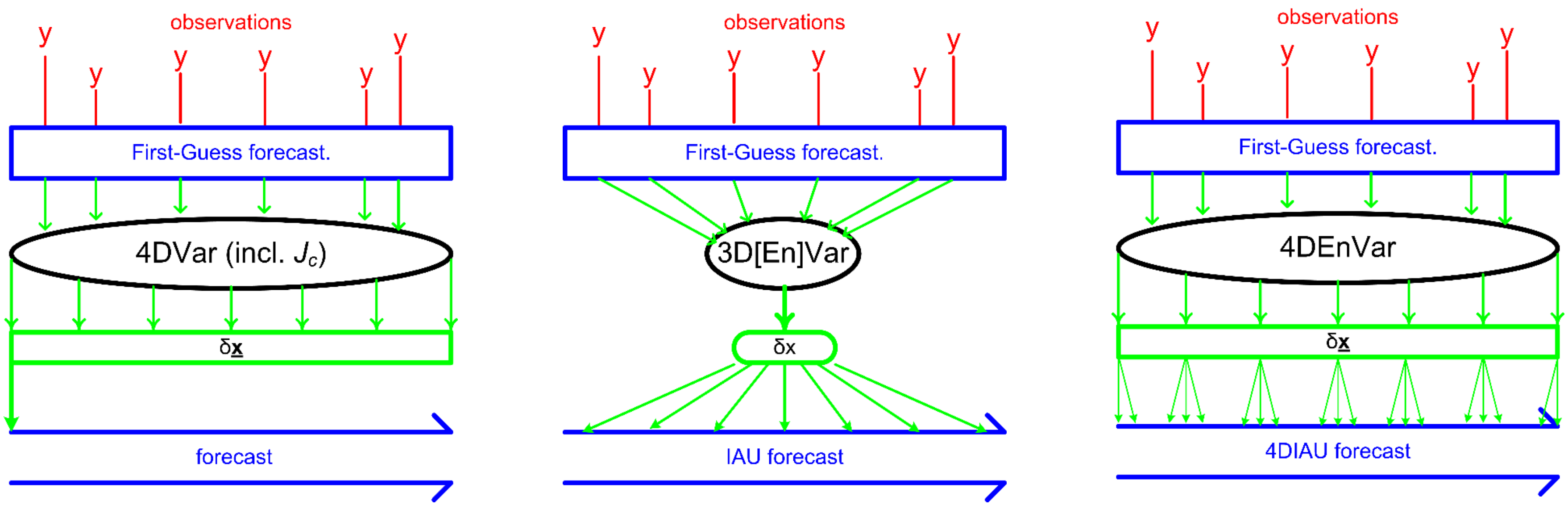
 Andrew Lorenc

Conclusions from 4D analysis increment study

1. The main error in our hybrid-4DEnVar (v hybrid-4DVar) is that the climatological covariance is used as in 3DVar.

2. 3D localisation not following the flow is not an important error for our 1200km localisation scale and 6hour window, but does become important for a 500km scale.

Initialization



4DVar's
$J_c = \frac{1}{2}\left(\mathbf{F}\delta\underline{\mathbf{x}}\right)^T \mathbf{G}^{-1}\left(\mathbf{F}\delta\underline{\mathbf{x}}\right)$
produces balanced increments by penalizing gravity waves.

IAU applied a related time-filter (Polavarapu *et al.*, 2004) while adding increments to model.

4DIAU has less time-filtering, but is effective at cancelling noise in the increment trajectory.

4DIAU – Initialisation

Lorenc *et al.* (2014) studied the simple 4DIAU method
– it works effectively for 4DEnVar.

4DIAU is used in operational 4DEnVar in

- EC (Canada) Buehner *et al.* (2015),
- NCEP (USA) (Kleist, personal communication).

The only problem is that it rules out an outer-loop.

Improving 4DEnVar

The maintenance and running costs of hybrid-4DVar are larger, so there is an incentive to improve hybrid-4DEnVar.

We need to reduce the weight on climatological $\mathbf{B}$ relative to the ensemble covariance.

We must first improve the ensemble covariances:

- **a bigger ensemble;**
- **better ensemble generation;**
- **better filtering of ensemble covariance, e.g. localization.**

Encouraging progress has been made in all of these.

Localisation

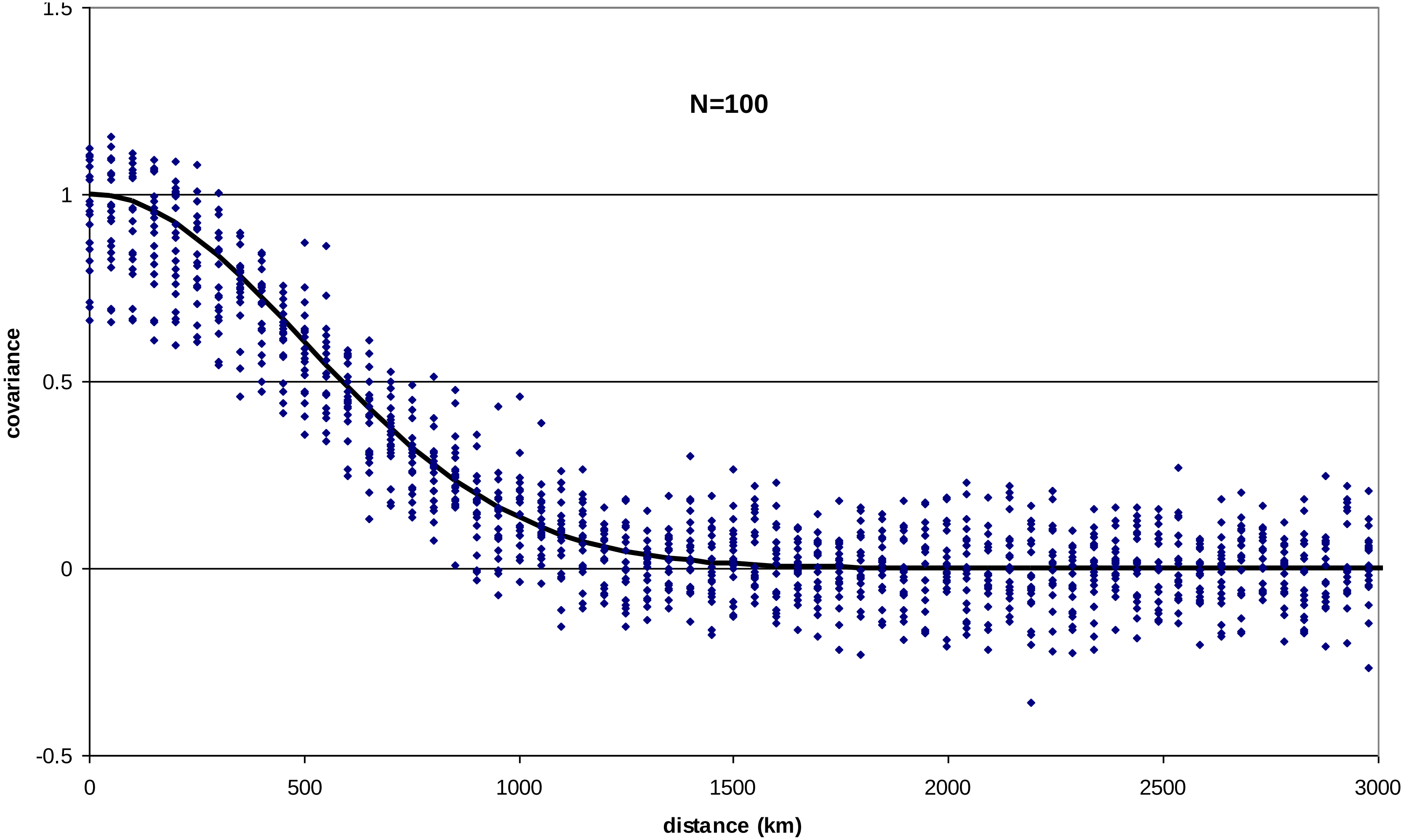
Ensemble covariance filtering

Covariance $\mathbf{B}$ is big! We need a large ensemble PLUS clever filtering to reduce sampling noise, based on 2 ideas:

- Assume some correlations are near zero, & localise: horizontal, vertical, spectral, transformed variables;
- Assume local homogeneity − apply smoothing: horizontal, rotational, and time.

Horizontal localisation

Errors in sampled ensemble covariances

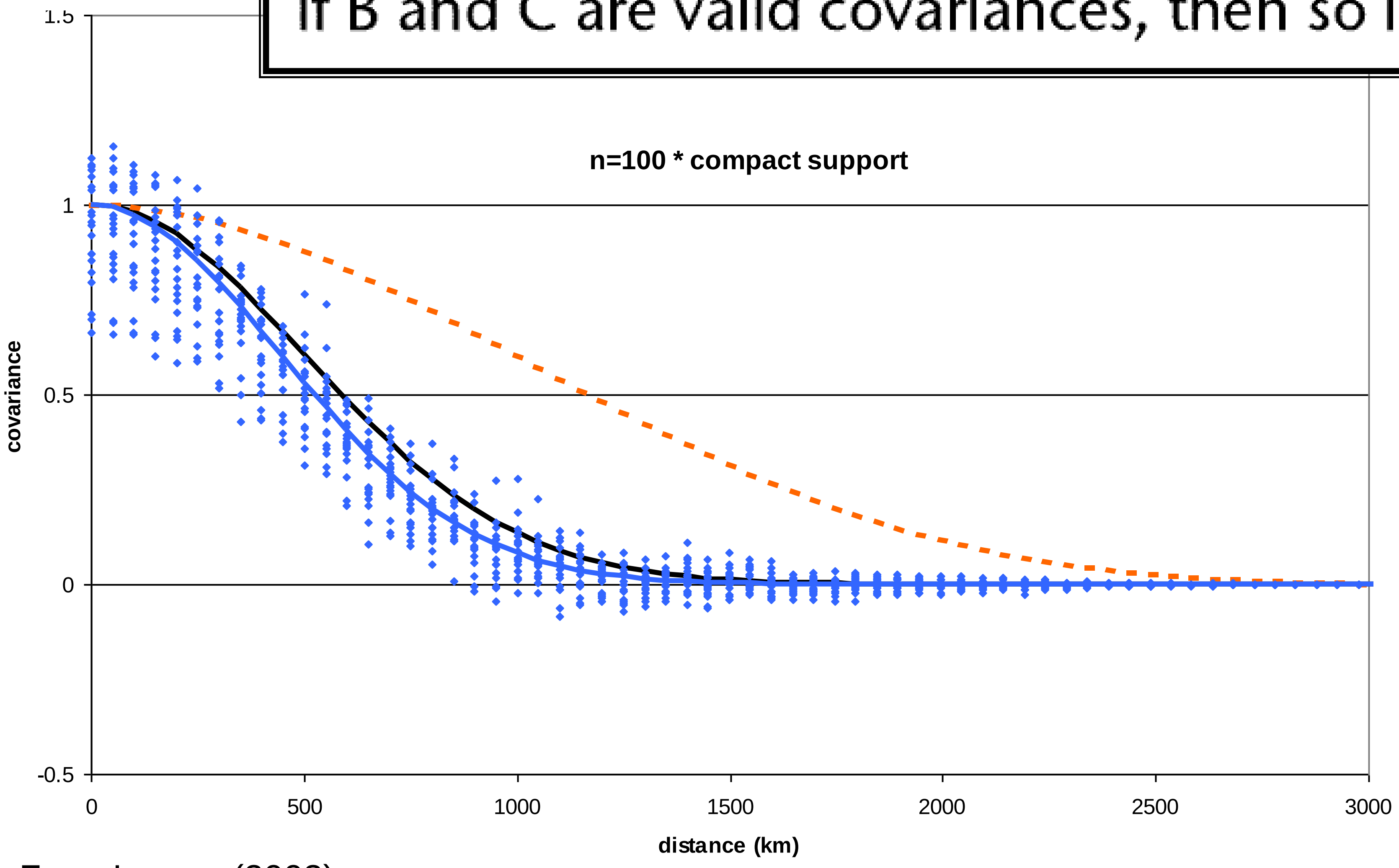


From Lorenc (2003)

The Schur Product

$\mathbf{A} = \mathbf{B} \circ \mathbf{C}$ such that $A_{i,j} = B_{i,j} C_{i,j}$.

If B and C are valid covariances, then so is A.



From Lorenc (2003)

Localisation – time-dimension

$$\text{3D: } \mathbf{P} = \mathbf{C} \circ \mathbf{X}\mathbf{X}^T$$

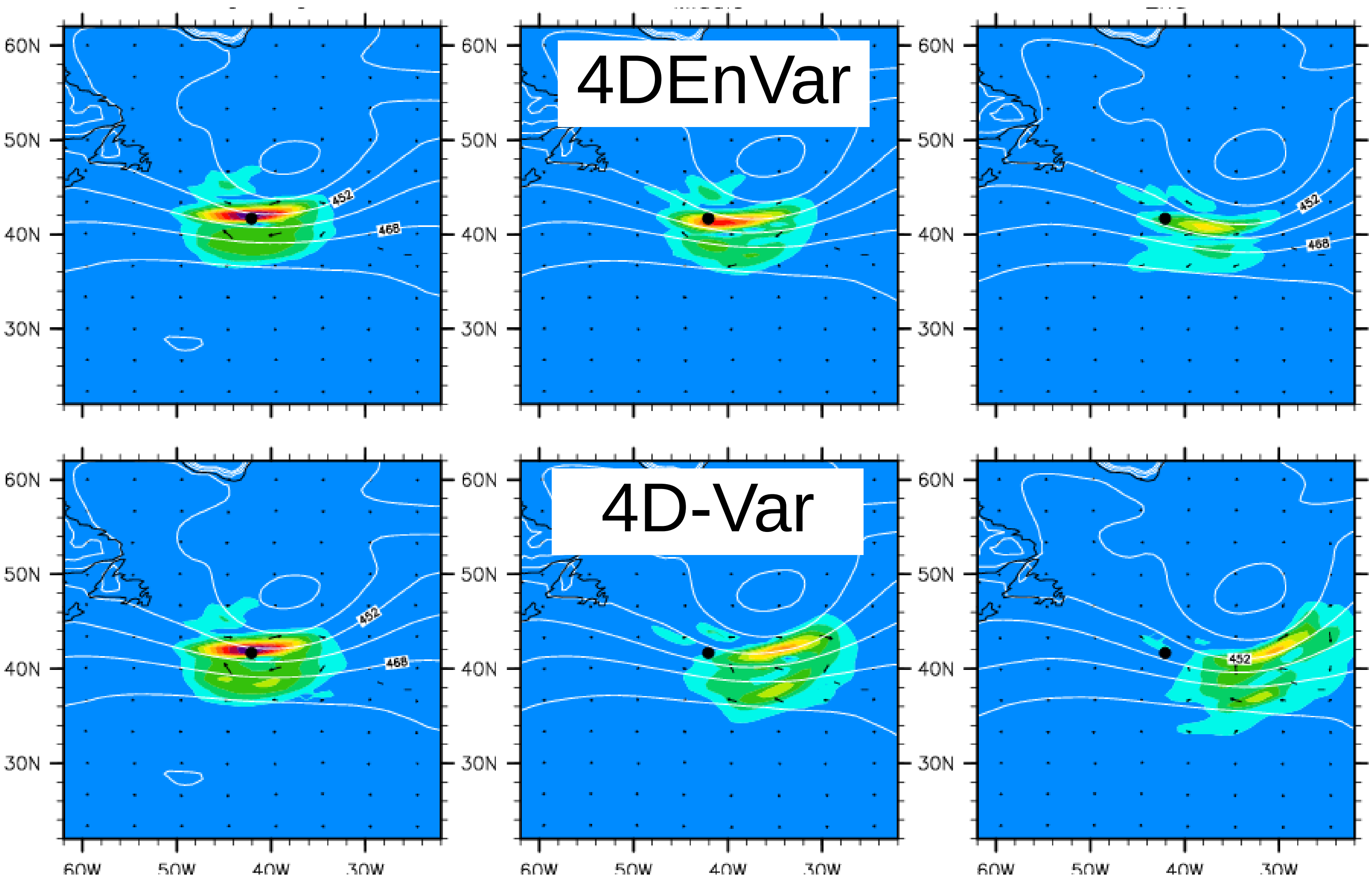
$$\text{4D: } \underline{\mathbf{P}} = \underline{\mathbf{C}} \circ \underline{\mathbf{X}}\underline{\mathbf{X}}^T$$

$\mathbf{C}$ is a correlation matrix, near 0 where the real covariance is small, otherwise near 1.

Nearly all 4DEnVar implementations have no time-localisation, so $\underline{\mathbf{C}} = \underline{\mathbf{I}}\mathbf{C}\underline{\mathbf{I}}^T$.

- Research ideas for time-varying localisation exist,
  e.g. Bishop and Hodyss (2011); Ota *et al.* (2013).
- The need for flow-following localisation depends on the time-window.
- *WARNING*: Time-localisation might give optimal estimate at one time,
  but NOT an optimal ongoing filter!

100% ensemble
500km localization scale



Localisation – transformed variables

Any linear transform of $\mathbf{X}$ gives an equally valid covariance.

So we can equally well localise using $\mathbf{P} = \mathbf{T}^{-1}\left(\mathbf{C} \circ \mathbf{T}\mathbf{X}\mathbf{X}^T\mathbf{T}^T\right)\mathbf{T}^{-T}$.

The Met Office EnVar localises transformed variables:

– this avoids the imbalance normally caused by localisation.

There is the option of localising between transformed variables

– this imposes balance relationships implicit in the transforms.

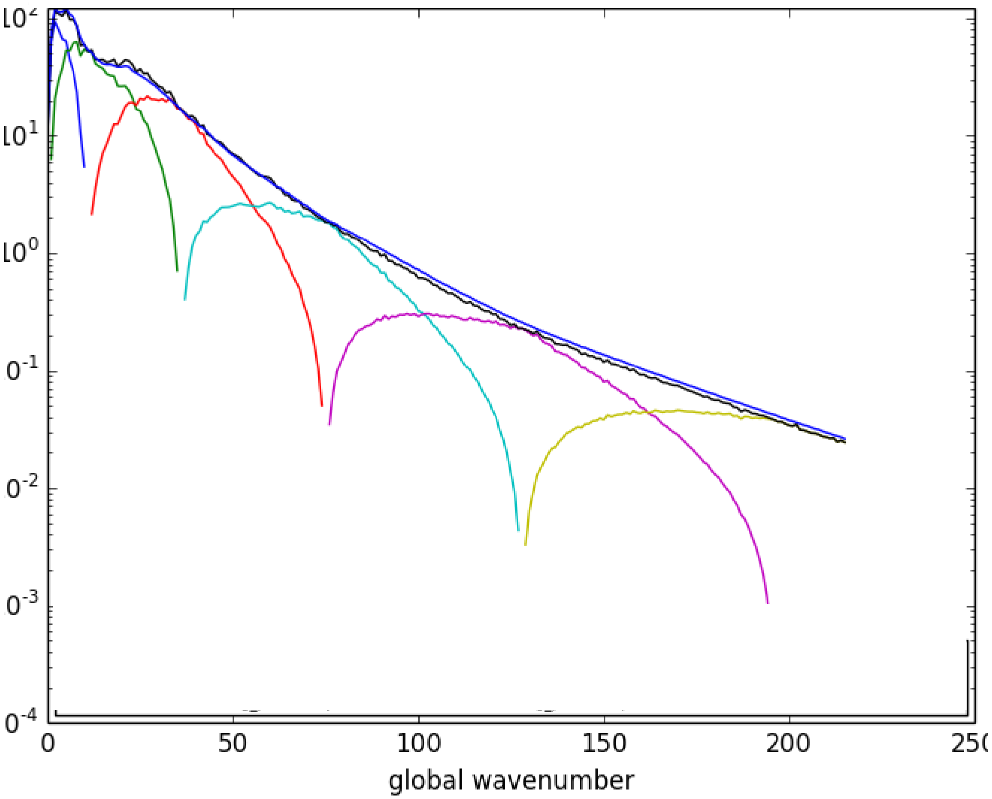
Buehner and Charron (2007); Buehner (2012) suggested spectral localisation;

– this has the effect of smoothing in space;

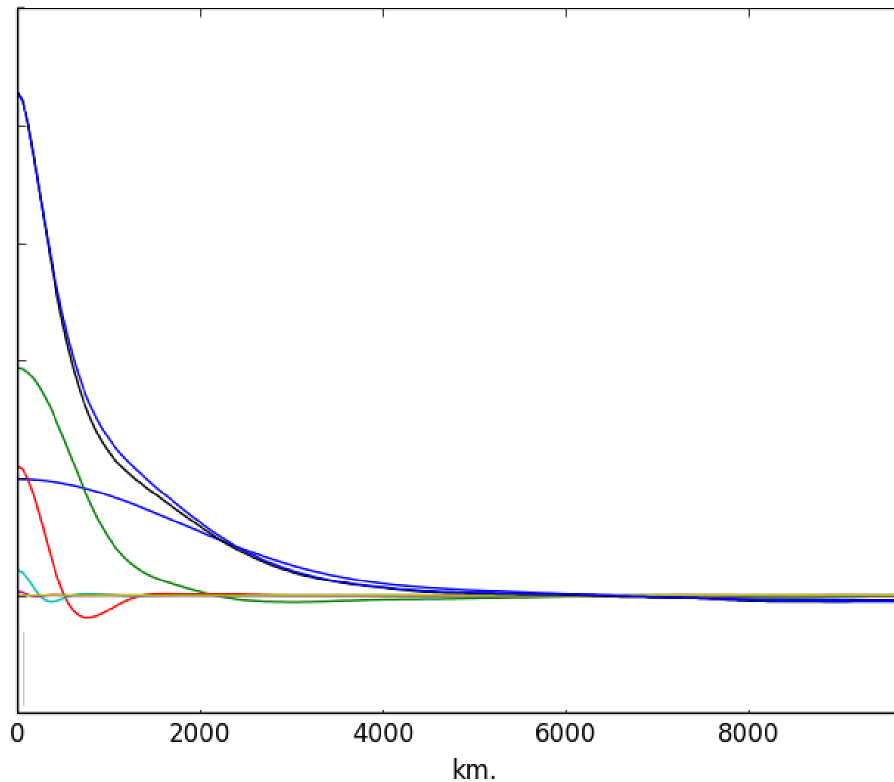
– the wavebands allow different horizontal localisations for each scale.

Spectral [waveband] localisation, of pressure at 4km

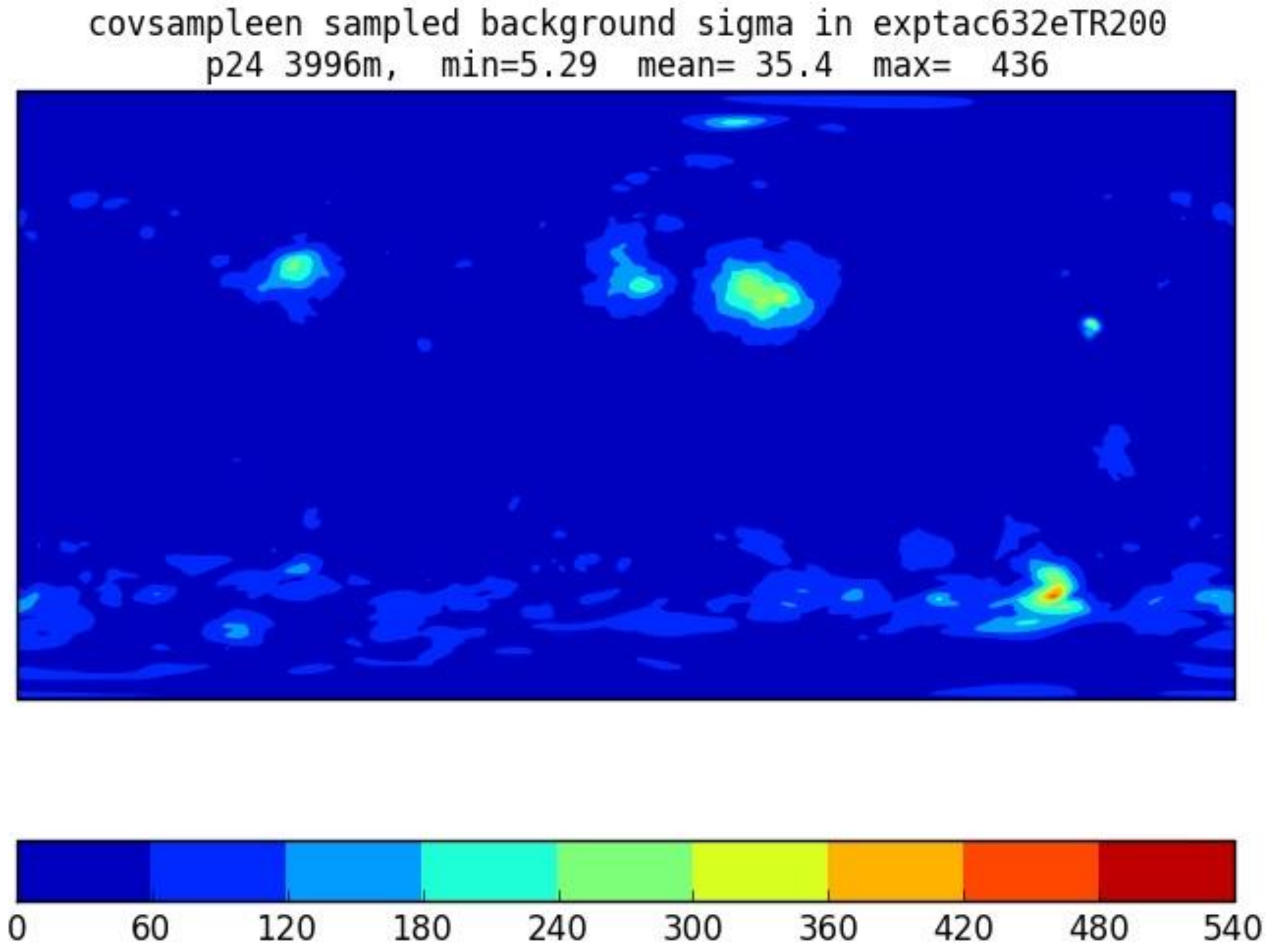
Input spectrum, 6 bands, sampled spectrum



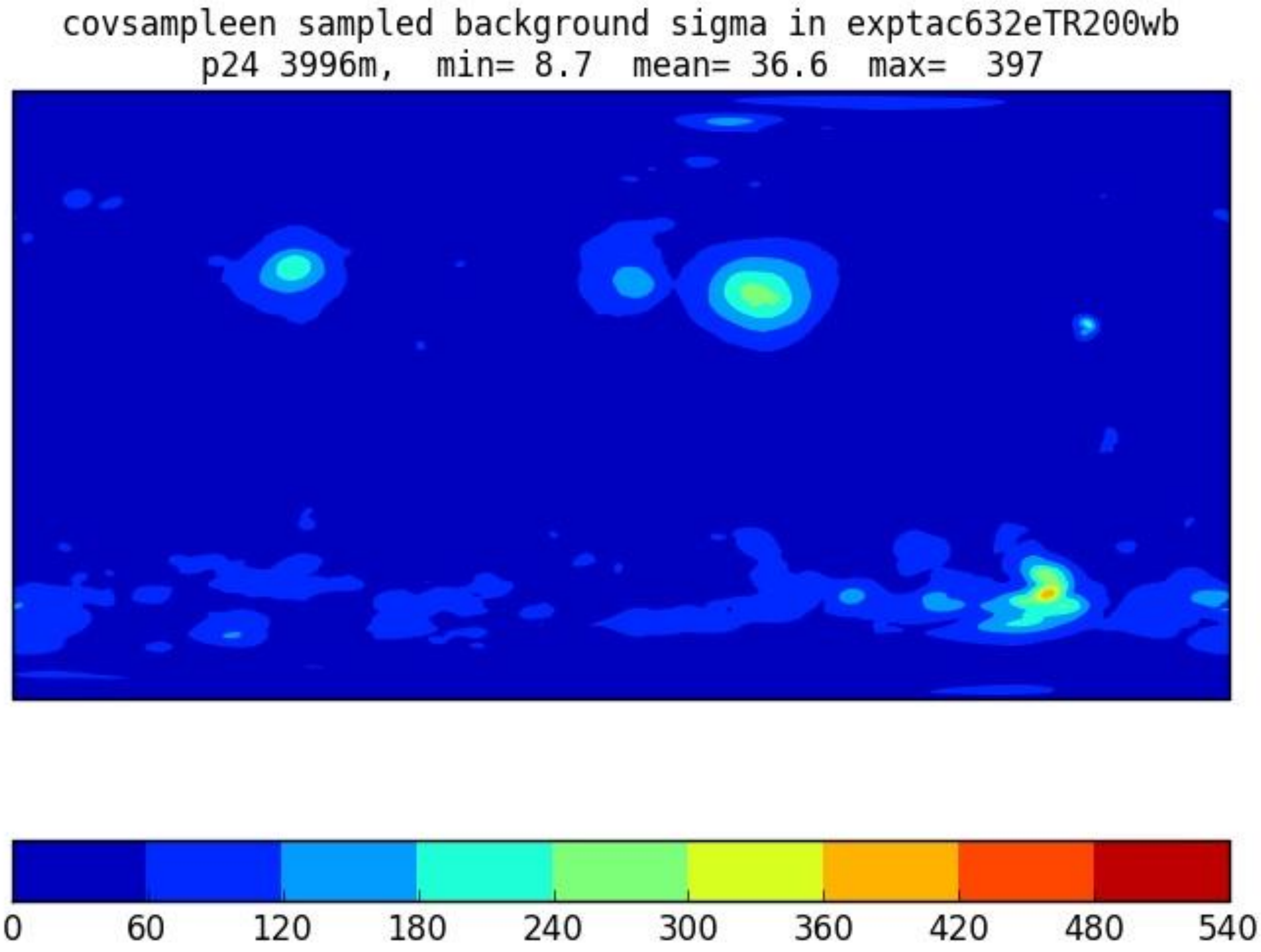
Implied global covariance functions



Ensemble spread in pressure at level 24 (~4km)



Spread, after localisation using 6 wavebands (~4km)



Localisation – different implementations

The EnVar schemes covered so far use an "$\boldsymbol{\alpha}$ control variable" (Lorenc, 2003) localisation to compensate for a small ensemble.

Another approach is to make extra members using eigenvectors of $\mathbf{C}$:

- This was used in early 4DEnVar (Liu *et al.*, 2009)
- and in spectral localisation (Buehner, 2012).

At what stage we localise makes a big difference:

- at start of time-window, before model – En-4DVar (Clayton *et al.*, 2013);
- EnKF schemes typically localise in ob-space after H;
  this is not as good (Campbell *et al.*, 2010) and cannot handle wavebands;
- the LETKF (Hunt *et al.*, 2007; Harlim and Hunt, 2007) localises by selecting obs outside the solution of the KF equation.

Plans

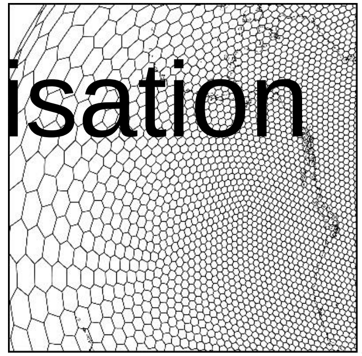
Comparison with hybrid-4DVar for global NWP

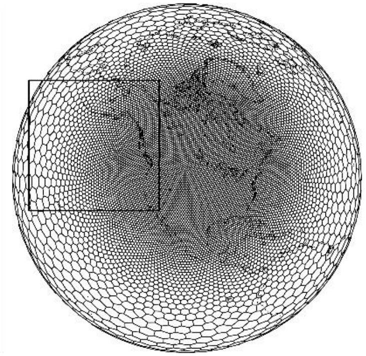
Hybrid-4DEnVar	**Hybrid-4DVar**
4D via use of ensemble trajectories. Only 3D use of climatological **B**.	4D via use of $\underline{\mathbf{M}}$ & $\underline{\mathbf{M}}^T$.
No forecast model inside algorithm, easy to add variables.	Needs special software for $\underline{\mathbf{M}}$ & $\underline{\mathbf{M}}^T$, effort needed to add variables.
Needs memory to store trajectories.	$\underline{\mathbf{M}}$ & $\underline{\mathbf{M}}^T$ have to be run each iteration.
Needs large ensemble and good localisation.	Needs good covariance model.

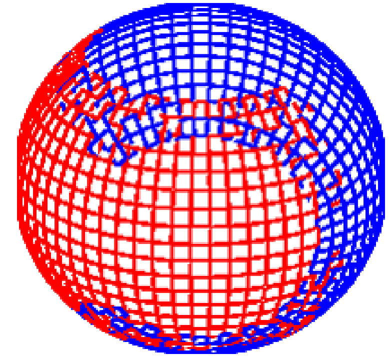
- The Met Office's operational hybrid-4DVar works well on current & next computer. But $\underline{\mathbf{M}}$ & $\underline{\mathbf{M}}^T$ are struggling with model changes and resolution increases.
- hybrid-4DEnVar will be the first method coded for use with the planned GungHo model on the massively parallel computer expected next decade.

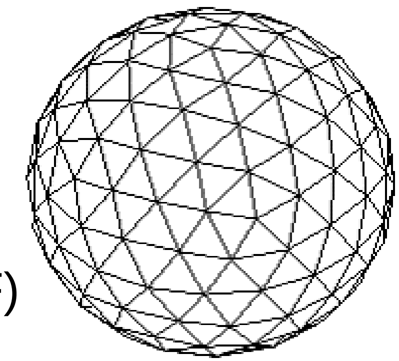
Met Office

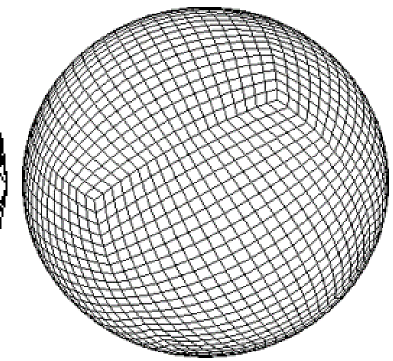
Parallelisation











4DVar has several potential problems looming in the next decade - their timing for each centres will depend on their computers and models:

1. Need new design to use millions of parallel threads, especially in sequential runs of linear (PF) and Adjoint models.

2. Forecast models are being redesigned to address this − a maintenance issue for the PF and Adjoint models.

4DEnVar is a simple solution, using the ensemble trajectories, pre-calculated in parallel, instead of the models inside 4DVar.

If Fourier filters and Poisson solvers are not available then the LETKF is an easier approach.

Comparison with EnKF for Convective−scale NWP

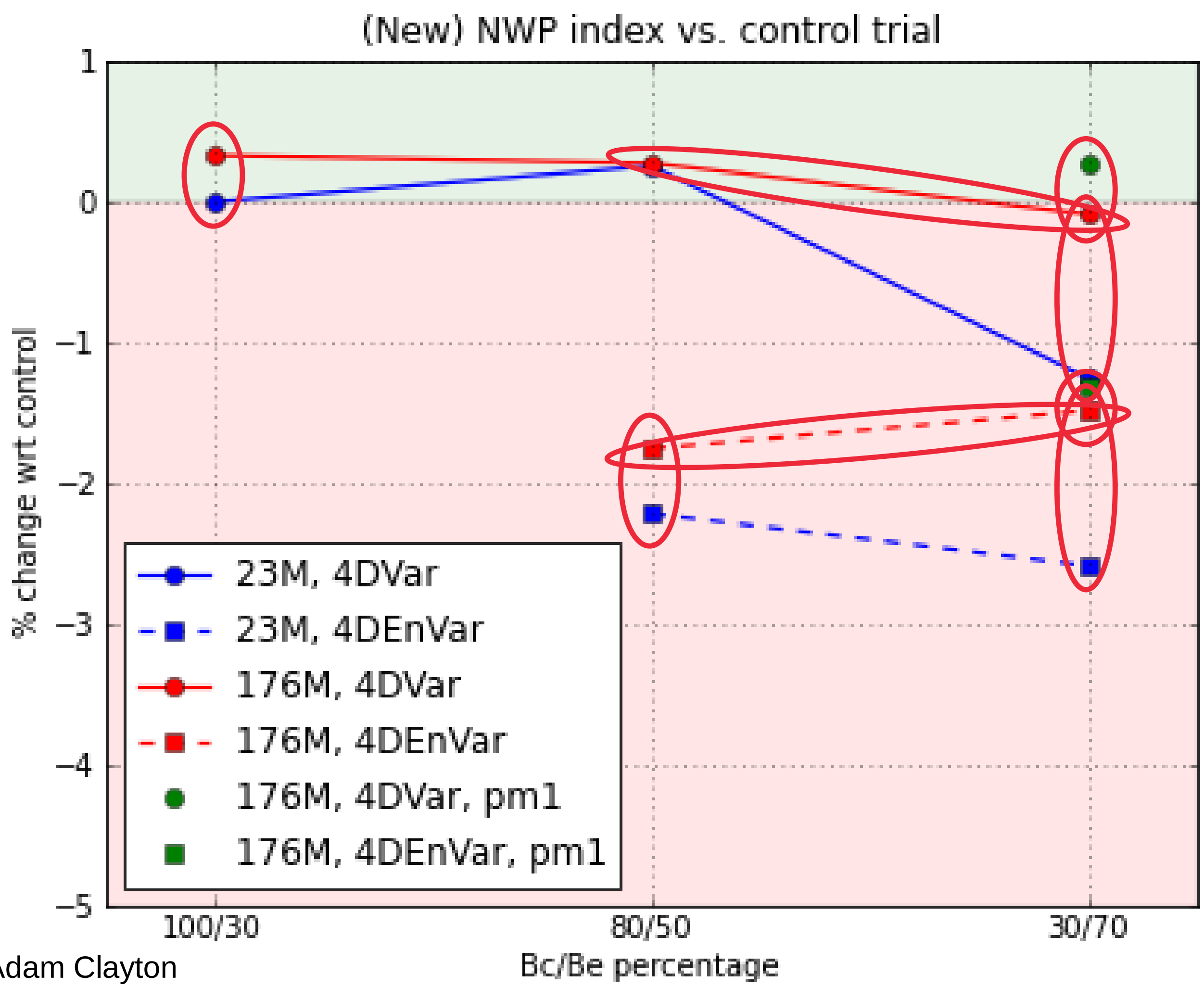
Hybrid-4DEnVar	EnKF
Needs transforms and filters of model fields, each iteration.	Works locally, using ensemble predictions of observations $H(\underline{\mathbf{x}}^b{}_k)$.
	Easy to build & cheap to run; cost small compared to ensemble forecasts.
Using wavebands, better for analysing a wide range of scales, including large scales from global ensemble. Can use hybrid with climatological **B**.	

- We cannot yet run a big enough ensemble of good enough forecasts to effectively sample background error covariance. Priority is on improving model & computer.
- Meanwhile Met Office is running 3DVar and developing 4DVar, with a small forecast ensemble via downscaling of the global ensemble.
- We will start experimenting with En-DA with a simple EnKF (concentrating on model forecasts and infrastructure). 4DEnVar is not yet planned.

How to create the ensemble?

- From a separate EnKF system. E.g.:
  - ➢Canada uses an independent EnKF (Houtekamer et al. 2014)
  - ➢Met Office MOGREPS (Bowler et al., 2008; Flowerdew and Bowler, 2011) uses a Localised ETKF re-centred on a deterministic analysis.
- From an Ensemble of 4DEnVar (EDA: Bonavita et al., 2012)
  - ➢We are experimenting with this, including a MeanPert algorithm to reduce cost.
  - ➢From a single EnVar's Hessian information: EVIL (Aulígné, 2012)
- Downscaling from a global ensemble
  - ➢Met Office experience with regional MOGREPS $\Rightarrow$ this is key process
  - ➢Canada's regional 4DEnVar uses the global ensemble (Caron et al., 2015)

Trials of increased ensemble size and weight



Modest improvement when increasing ensemble size

Much larger improvement when ensemble weight is high

4DVar performs worse with high ensemble weight, 4DEnVar performs better

Using ensemble modes from the wrong time brings a small benefit

Adam Clayton

4DEnVar: Summary of Talk

- Design

4D using ensemble $\Rightarrow$ hybrid-4DVar / hybrid-4DEnVar / EnKF

- Comparison with 4DVar

4DEnVar time propagation OK except in hybrid.

- Localisation & filtering of ensemble covariance

Space, transformed, spectral (wavebands), time, how.

- Plans

Method (global & convective), MPP, getting ensemble, size

Questions and answers

LETKF solves KF equations separately for each grid-point, with local observations.

Use the matrix of ensemble model-ob perturbations calculated using nonlinear H:

$$\underline{\mathbf{y}}'_k = \frac{1}{\sqrt{N-1}}\left(\underline{H}\left(\underline{\mathbf{x}}_k^b\right) - \overline{\underline{H}\left(\underline{\mathbf{x}}^b\right)}\right)$$

$$\underline{\mathbf{Y}}^b = \left[\begin{array}{ccc} \underline{\mathbf{y}}'_1 & \cdots & \underline{\mathbf{y}}'_N \end{array}\right]$$

ETKF for mean analysis

$$\delta\underline{\mathbf{x}} = \underline{\mathbf{X}}^b\mathbf{w}$$

$$\mathbf{w} = \tilde{\mathbf{P}}^a\left(\underline{\mathbf{Y}}^b\right)^T\mathbf{R}^{-1}\left(\underline{\mathbf{y}}^o - \underline{H}\left(\underline{\mathbf{x}}^b\right)\right)$$

The ensemble-space matrix inversion is solved directly

$$\tilde{\mathbf{P}}^a = \left[\mathbf{I} + \left(\underline{\mathbf{Y}}^b\right)^T\mathbf{R}^{-1}\underline{\mathbf{Y}}^b\right]^{-1}$$

SQRT-filter for the analysis pertubations

$$\underline{\mathbf{X}}^a = \left(\tilde{\mathbf{P}}^a\right)^{1/2}\underline{\mathbf{X}}^b$$

Each point's $\mathbf{w}$ is a row of matrix whose columns are $\boldsymbol{\alpha}$

$$\mathbf{A} = \left[\begin{array}{ccc} \boldsymbol{\alpha}'_1 & \cdots & \boldsymbol{\alpha}'_N \end{array}\right] \propto \left[\begin{array}{c} \mathbf{w}_1^T \\ \vdots \\ \mathbf{w}_{Npt}^T \end{array}\right]$$

Hunt *et al.* (2007); Harlim and Hunt (2007) apply the factor $1/\sqrt{N-1}$ to $\mathbf{w}$ & $\boldsymbol{\alpha}$ rather than to $\mathbf{X}^b$.

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My related talks:

Comparing ensemble-variational assimilation methods for NWP: Can hybrid-4DEnVar match hybrid-4DVar? WWOSC, Montreal, August 2014. https://www.wmo.int/pages/prog/arep/wwrp/new/wwosc/documents/Lorenc_4DEnVar_4DVar.pdf

Advances in data assimilation techniques and their relevance to satellite data assimilation. ECMWF Seminar on Use of Satellite Observations in NWP,8-12 September 2014. http://www.ecmwf.int/sites/default/files/Lorenc_AdvancesDAsatellites.pdf