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Developments of Variational Data Assimilation

ECMWF Seminar on *Data Assimilation for Atmosphere and Ocean*.

Sept 2011. *Andrew Lorenc*

Content

1. Historical context
2. Reminder of 4D-Var derivation
3. Developments in error modelling
4. Coping with Butterflies
5. 4D-Ensemble-Var

I only have time to discuss general principles.
There will be more detail on many topics in later seminars.

Historical Background:

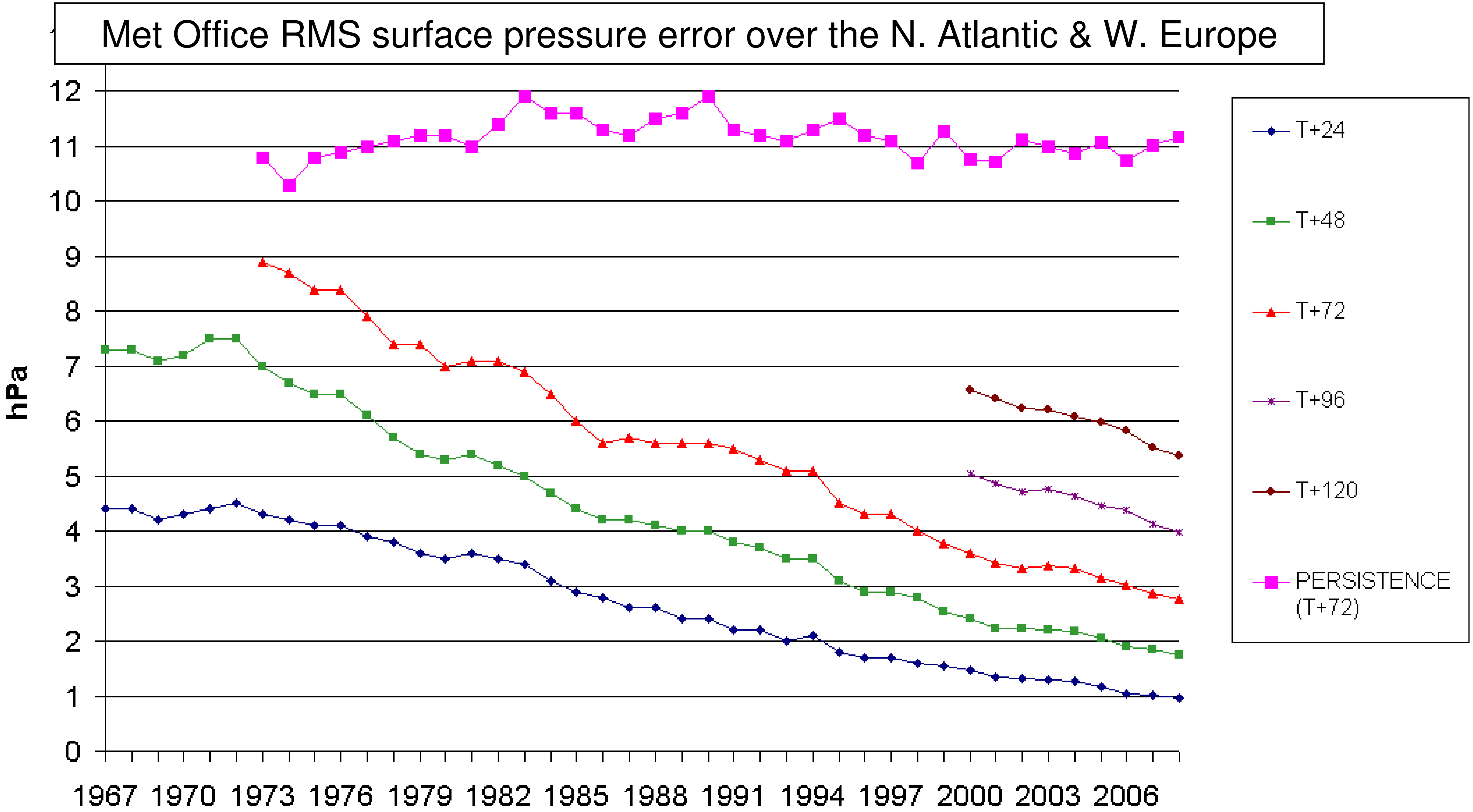
What has been important for getting the best NWP forecast? *(over last 3 decades)*

NWP systems are improving by 1 day of predictive skill per decade. This has been due to:

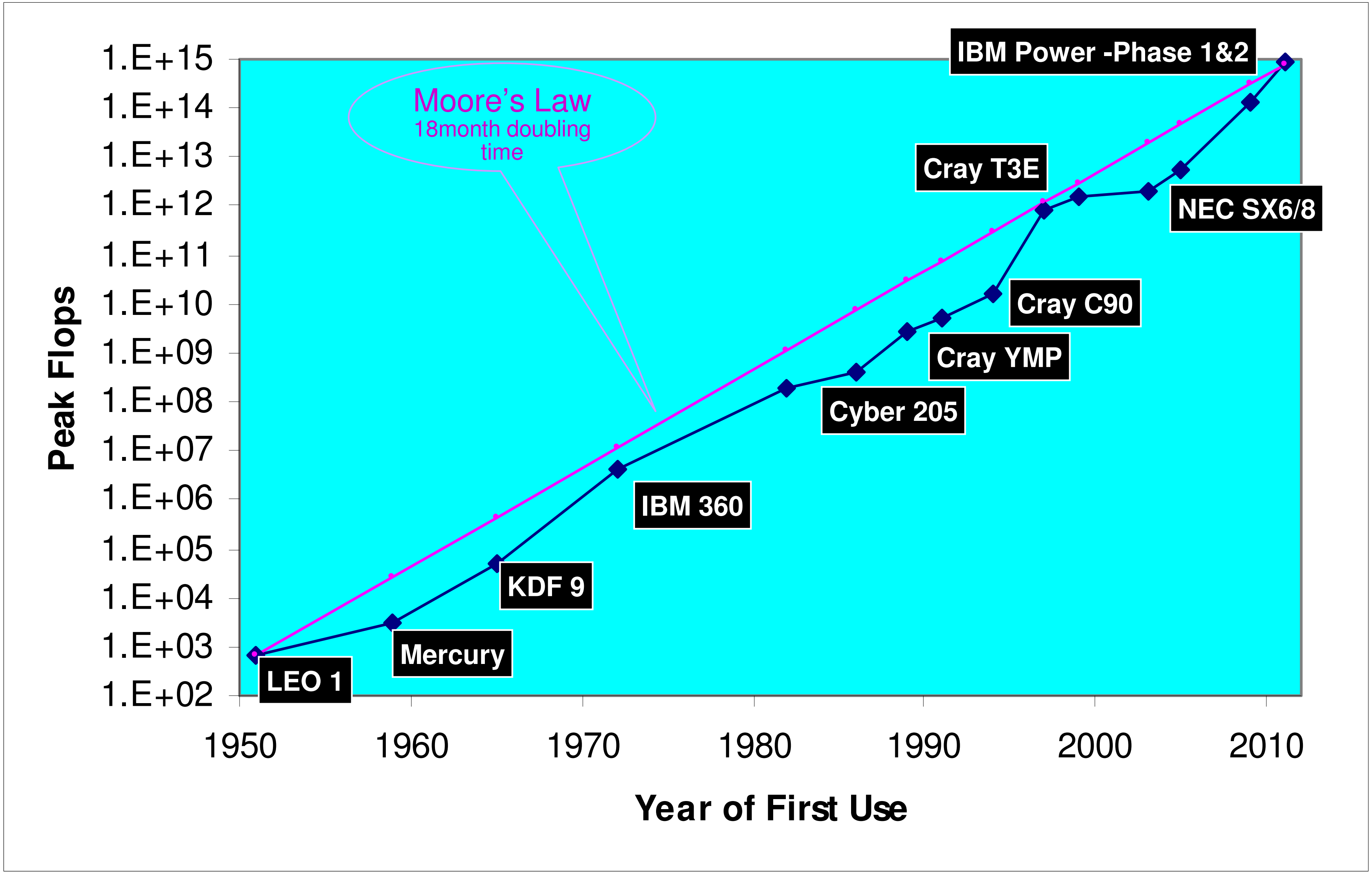
1. *Model improvements, especially resolution.*
2. *Careful use of forecast & observations, allowing for their information content and errors.*
   Achieved by variational assimilation e.g. of satellite radiances. (Simmons & Hollingsworth 2002)
3. *Advanced assimilation using forecast model: 4D-Var.*
4. *Better observations.*

Performance Improvements

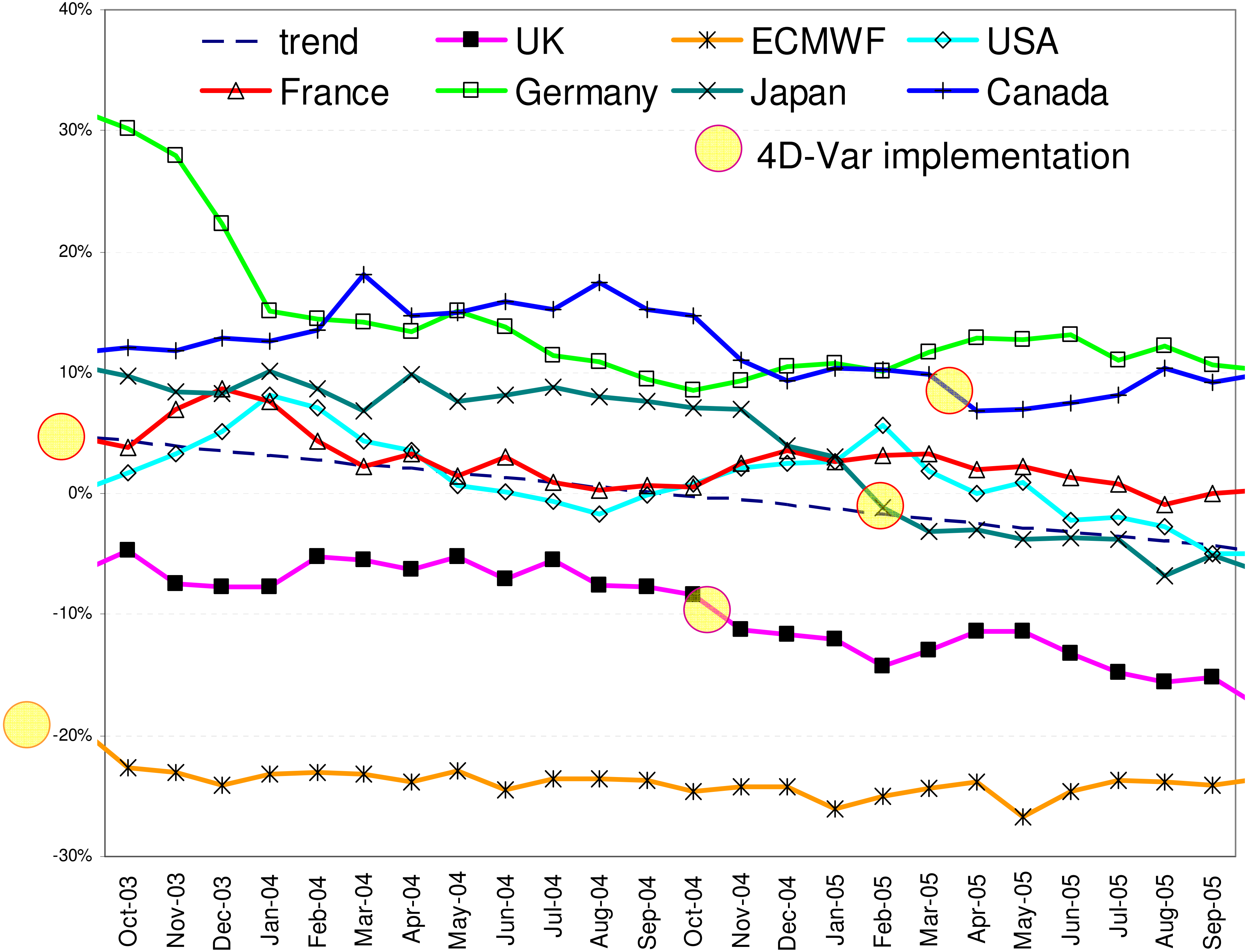
“Improved by about a day per decade”



60 Years of Met Office Computers



RMS errors with mean intra-annual variability removed



Impact of different observing systems.

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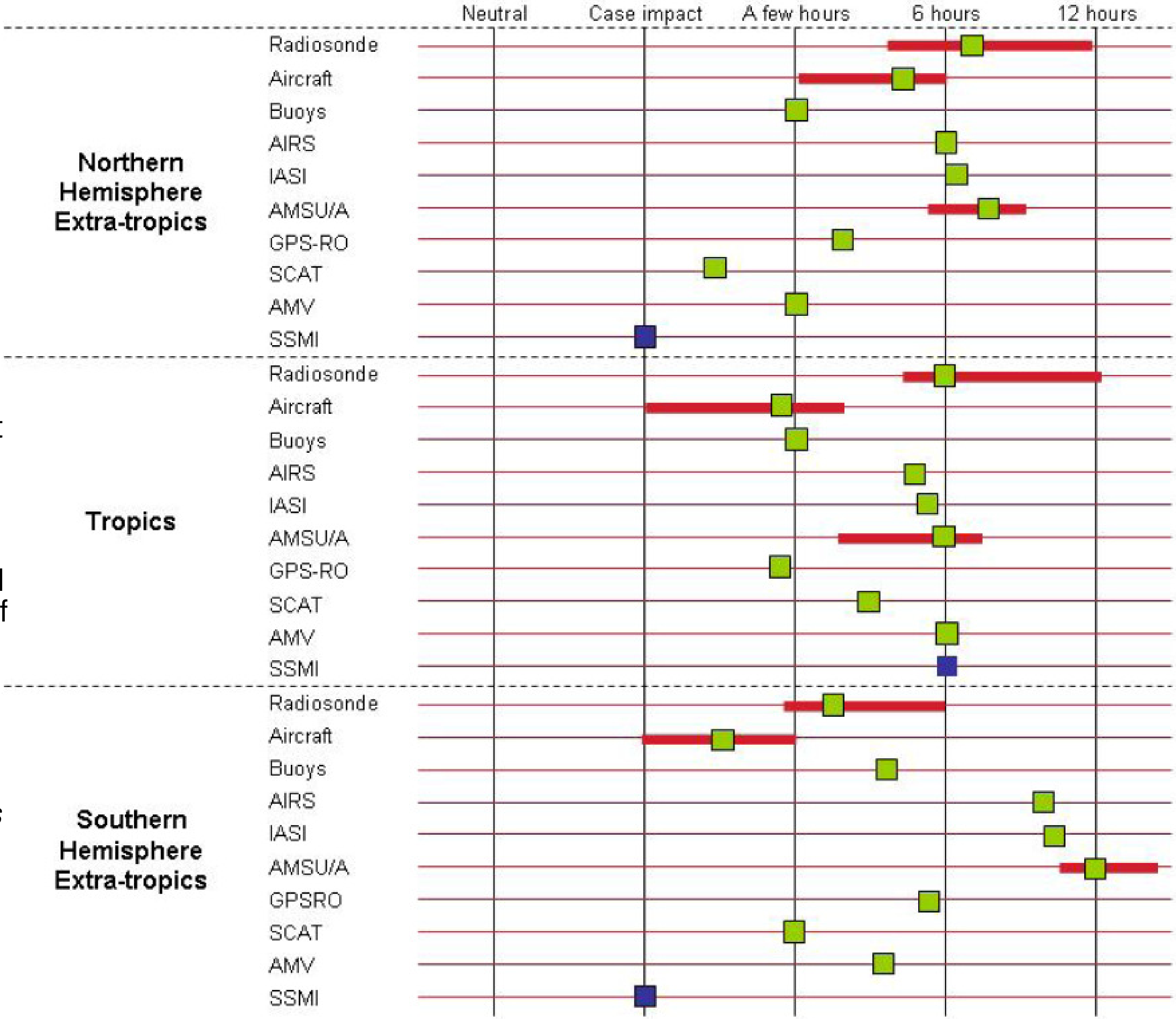
Current contributions of parts of the existing observing system to the large-scale forecast skill at short and medium-range. The green colour means the impact is mainly on the mass and wind field. The blue colour means the impact is mainly on humidity field. The contribution is primarily measured on large-scale upper-air fields. The red horizontal bars give an indication of the spread of results among the different impact studies so far available.

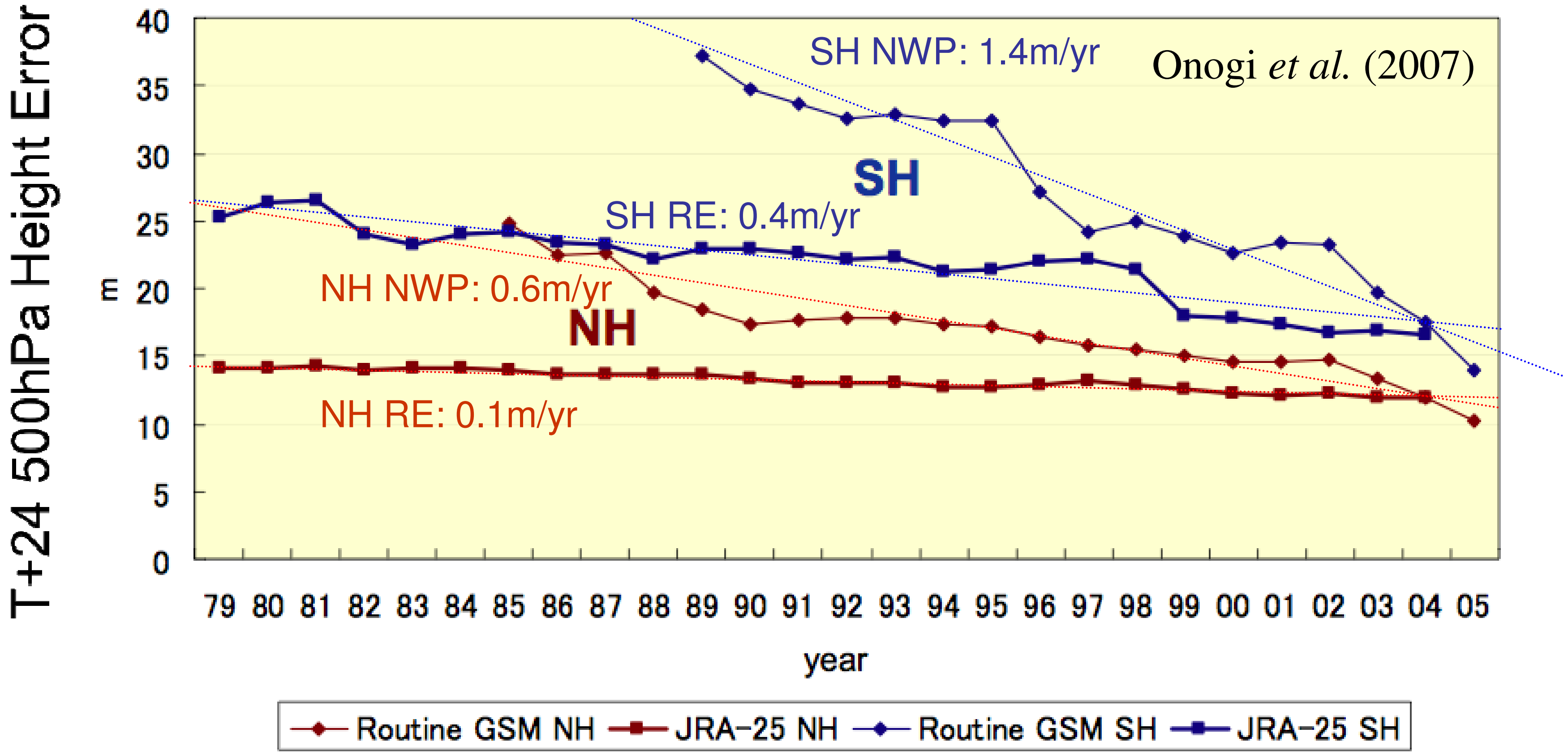
Fourth WMO Workshop on the Impact of Various Observing Systems on NWP.
Geneva, Switzerland, 19-21 May 2008



JMA NWP/Reanalysis performance

NWP=Changing model/DA *Reanalysis=Fixed model/DA*

Observation network evolves in both NWP and reanalysis



- Conclude: Most forecast benefit due to forecast/DA not more observations.
- Caveat: Not true for all metrics (e.g. precipitation shows bigger impact of obs).

Historical Background: Continuing Improvement of a Complex System

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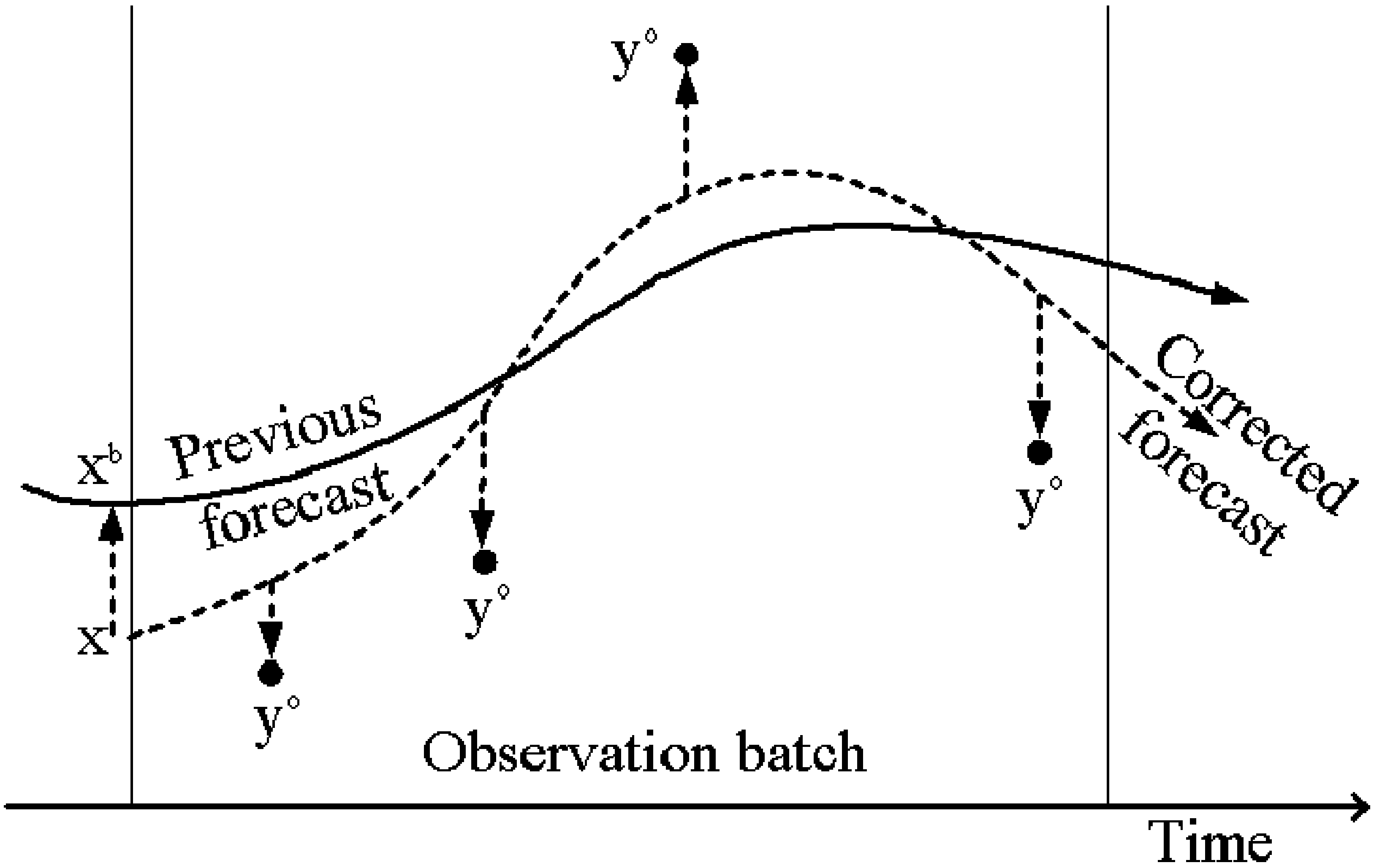
- NWP improvements are due to a synergistic combination of improvements of forecast model, DA and observations.
  - Each helps the other.
- Total NWP system is very large, complex and expensive.
  - We cannot expect to understand it completely as a single entity.
  - We cannot afford thorough testing of each improvement.
- Best to base each improvement of scientific insight and mathematical analysis of one component.
  - With belief (checked by testing) that theoretically better parts will eventually give a better system.

2. Reminder of 4D-Var Derivations

- **Deterministic**: fitting a model trajectory to observations.
- **Statistical**: Bayesian combination of model and observations, allowing for errors in each.

Simple 4D-Var, as a least-squares best fit of a deterministic model trajectory to observations



The deterministic 4D-Var equations

Bayesian posterior pdf. $$P\left(\mathbf{x}\middle|\underline{\mathbf{y}}^o\right) \propto P(\mathbf{x})\,P\left(\underline{\mathbf{y}}^o\middle|\mathbf{x}\right)$$

Assume Gaussians

$$P(\mathbf{x}) \propto \exp\left(-\tfrac{1}{2}\left(\mathbf{x}-\mathbf{x}^b\right)^T \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right)\right)$$

$$P\left(\underline{\mathbf{y}}^o\middle|\mathbf{x}\right) = P\left(\underline{\mathbf{y}}^o\middle|\underline{\mathbf{y}}\right) \propto \exp\left(-\tfrac{1}{2}\left(\underline{\mathbf{y}}-\underline{\mathbf{y}}^o\right)^T \underline{\mathbf{R}}^{-1}\left(\underline{\mathbf{y}}-\underline{\mathbf{y}}^o\right)\right)$$

But nonlinear model makes pdf non-Gaussian:
full pdf is too complicated to be allowed for.

$$\underline{\mathbf{y}} = \underline{H}\left(\underline{M}(\mathbf{x})\right)$$

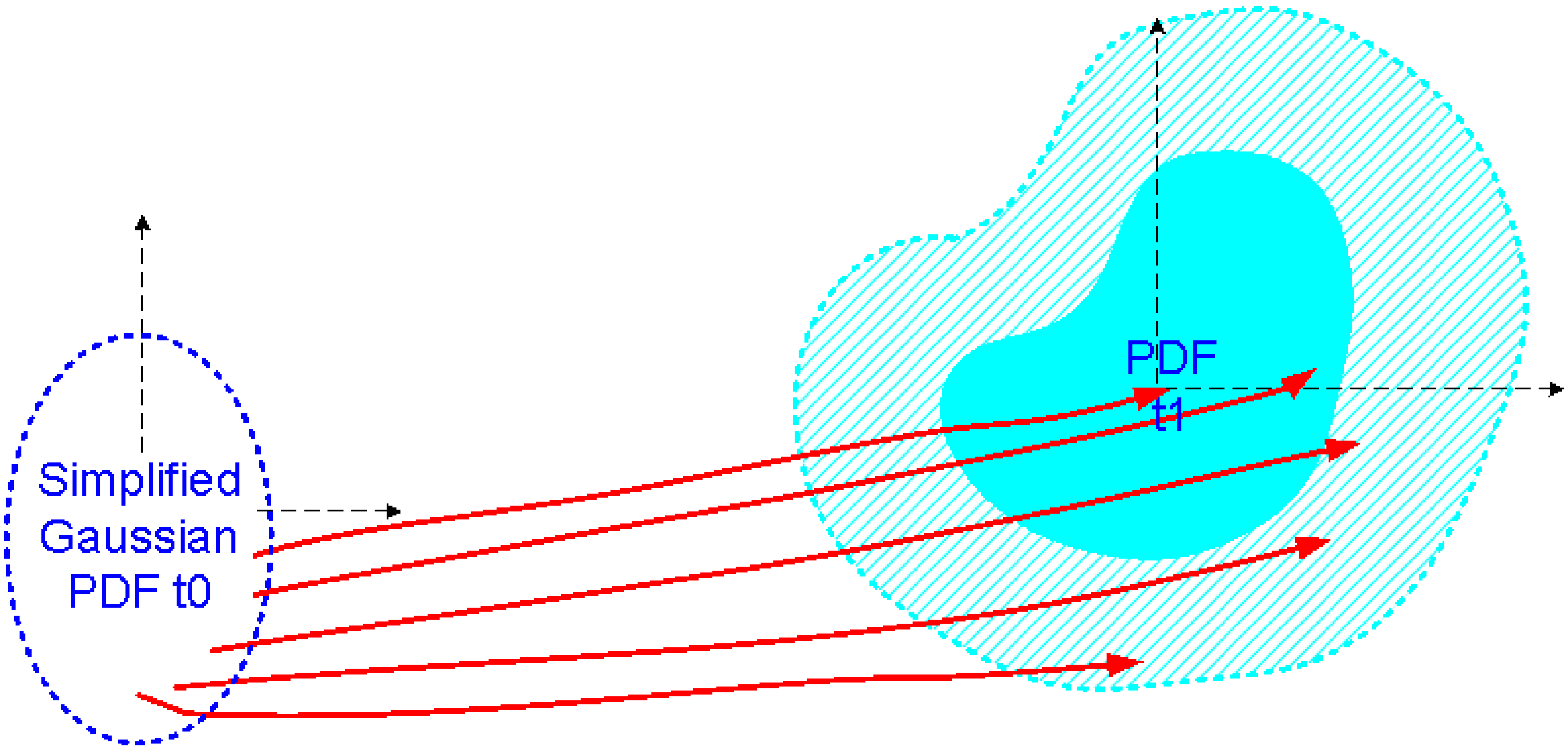
So seek mode of pdf by finding minimum of penalty function

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

$$\nabla_{\mathbf{x}} J(\mathbf{x}) = \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^b\right) + \underline{\mathbf{M}}^*\underline{\mathbf{H}}^*\mathbf{R}^{-1}\left(\underline{\mathbf{y}}-\underline{\mathbf{y}}^o\right)$$

Notation (to avoid summations over time): variables are 4D, operators produce 4D results.

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,
optionally augmented by a model error correction term.

When does deterministic 4D-Var using "automatic" adjoint methods not work?

Thermostats: - Fast processes which are modulated to maintain a longer-time-scale "balance" (e.g. boundary layer fluxes).

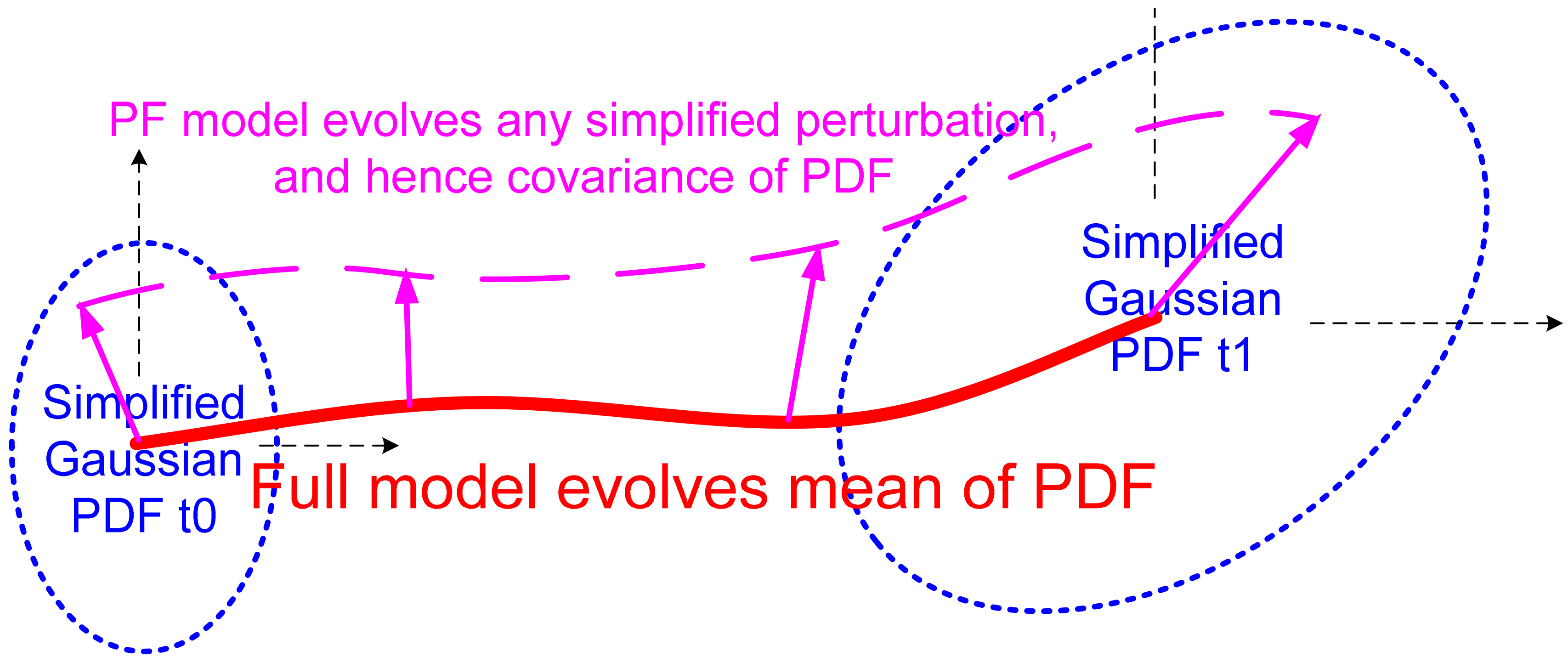
Limits to growth: - Fast processes which in a nonlinear model are limited by some available resource (e.g. evaporation of raindrops).

Butterflies: - Fast processes which are not predictable over a long 4D-Var time-window. (e.g. eddies with short space- & time-scales).

Observations of intermittent processes: - If something (e.g. a cloud or rain) is missing from a state, then the gradient does not say what to do to make it appear.

These are fundamental atmospheric processes – it is impossible to write a good NWP model without representing them.

Statistical, incremental 4D-Var



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

4D analysis increment is a trajectory of the PF model, optionally augmented by a model error correction term.

Statistical 4D-Var - equations

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Independent, Gaussian background and model errors $\Rightarrow$ non-Gaussian pdf for general $\mathbf{y}$:

$$P\left(\delta\mathbf{x},\delta\underline{\boldsymbol{\eta}}\middle|\underline{\mathbf{y}}^{o}\right)\propto\exp\left(-\tfrac{1}{2}\left(\delta\mathbf{x}-\left(\mathbf{x}^{b}-\mathbf{x}^{g}\right)\right)^{T}\mathbf{B}^{-1}\left(\delta\mathbf{x}-\left(\mathbf{x}^{b}-\mathbf{x}^{g}\right)\right)\right)$$
$$\exp\left(-\tfrac{1}{2}\left(\delta\underline{\boldsymbol{\eta}}+\underline{\boldsymbol{\eta}}^{g}\right)^{T}\underline{\mathbf{Q}}^{-1}\left(\delta\underline{\boldsymbol{\eta}}+\underline{\boldsymbol{\eta}}^{g}\right)\right)$$
$$\exp\left(-\tfrac{1}{2}\left(\underline{\mathbf{y}}-\underline{\mathbf{y}}^{o}\right)^{T}\underline{\mathbf{R}}^{-1}\left(\underline{\mathbf{y}}-\underline{\mathbf{y}}^{o}\right)\right)$$

Incremental linear approximations in forecasting model predictions of observed values converts this to an approximate Gaussian pdf:

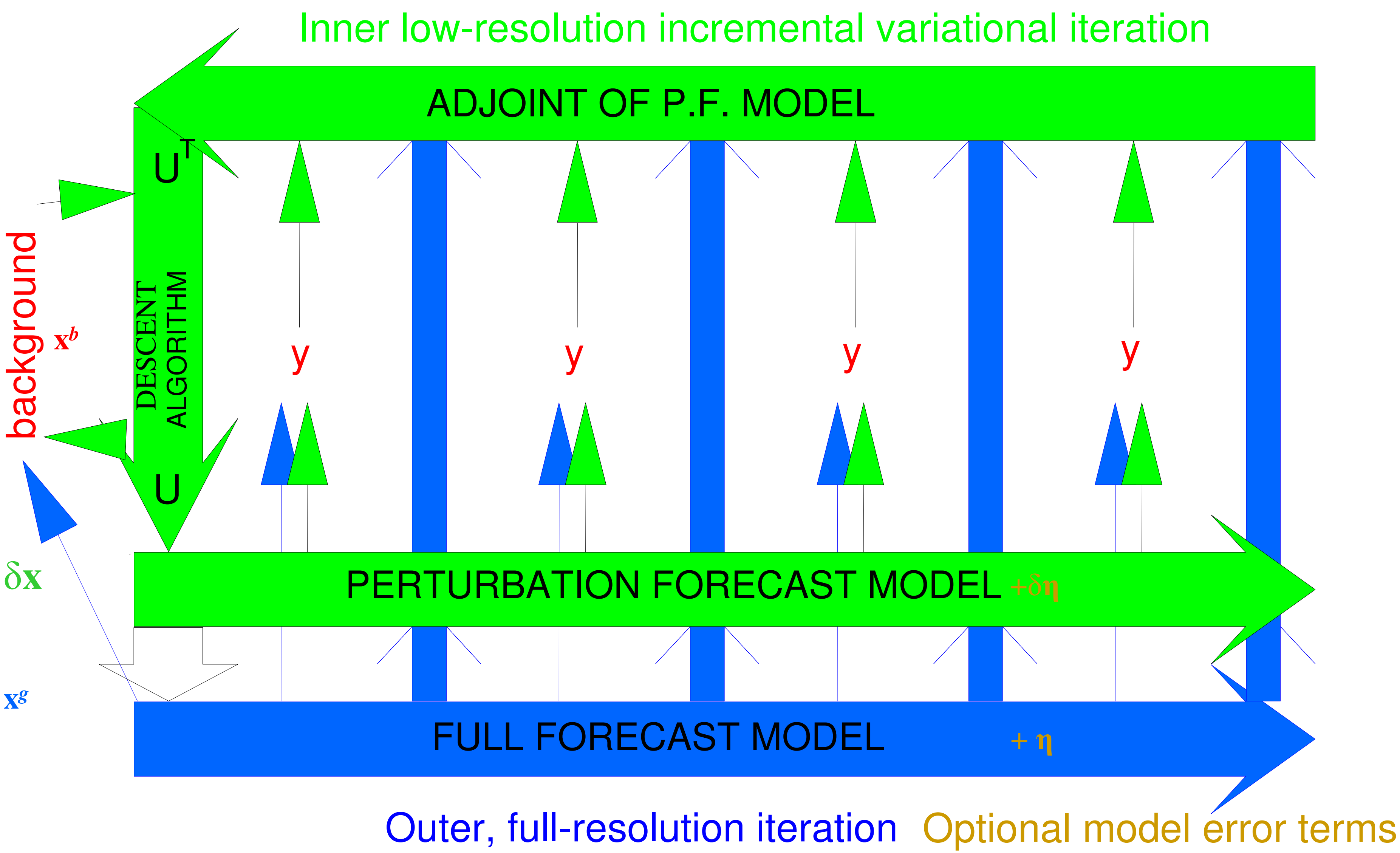
$$\underline{\mathbf{y}}=\underline{\tilde{\mathbf{H}}}\underline{\tilde{\mathbf{M}}}\left(\delta\mathbf{x},\underline{\boldsymbol{\eta}}\right)+\underline{\bar{H}}\left(\underline{\bar{M}}\left(\mathbf{x}^{g},\underline{\boldsymbol{\eta}}^{g}\right)\right)$$

The mean of this approximate pdf is identical to the mode, so it can be found by minimising:

$$J\left(\delta\mathbf{x},\delta\underline{\boldsymbol{\eta}}\right)=\tfrac{1}{2}\left(\delta\mathbf{x}-\left(\mathbf{x}^{b}-\mathbf{x}^{g}\right)\right)^{T}\mathbf{B}^{-1}\left(\delta\mathbf{x}-\left(\mathbf{x}^{b}-\mathbf{x}^{g}\right)\right)$$
$$+\tfrac{1}{2}\left(\delta\underline{\boldsymbol{\eta}}+\underline{\boldsymbol{\eta}}^{g}\right)^{T}\underline{\mathbf{Q}}^{-1}\left(\delta\underline{\boldsymbol{\eta}}+\underline{\boldsymbol{\eta}}^{g}\right)$$
$$+\tfrac{1}{2}\left(\underline{\mathbf{y}}-\underline{\mathbf{y}}^{o}\right)^{T}\underline{\mathbf{R}}^{-1}\left(\underline{\mathbf{y}}-\underline{\mathbf{y}}^{o}\right)$$

Lorenc (2003a)

Incremental 4D-Var with Outer Loop



Testing PF model for use in 4D-Var

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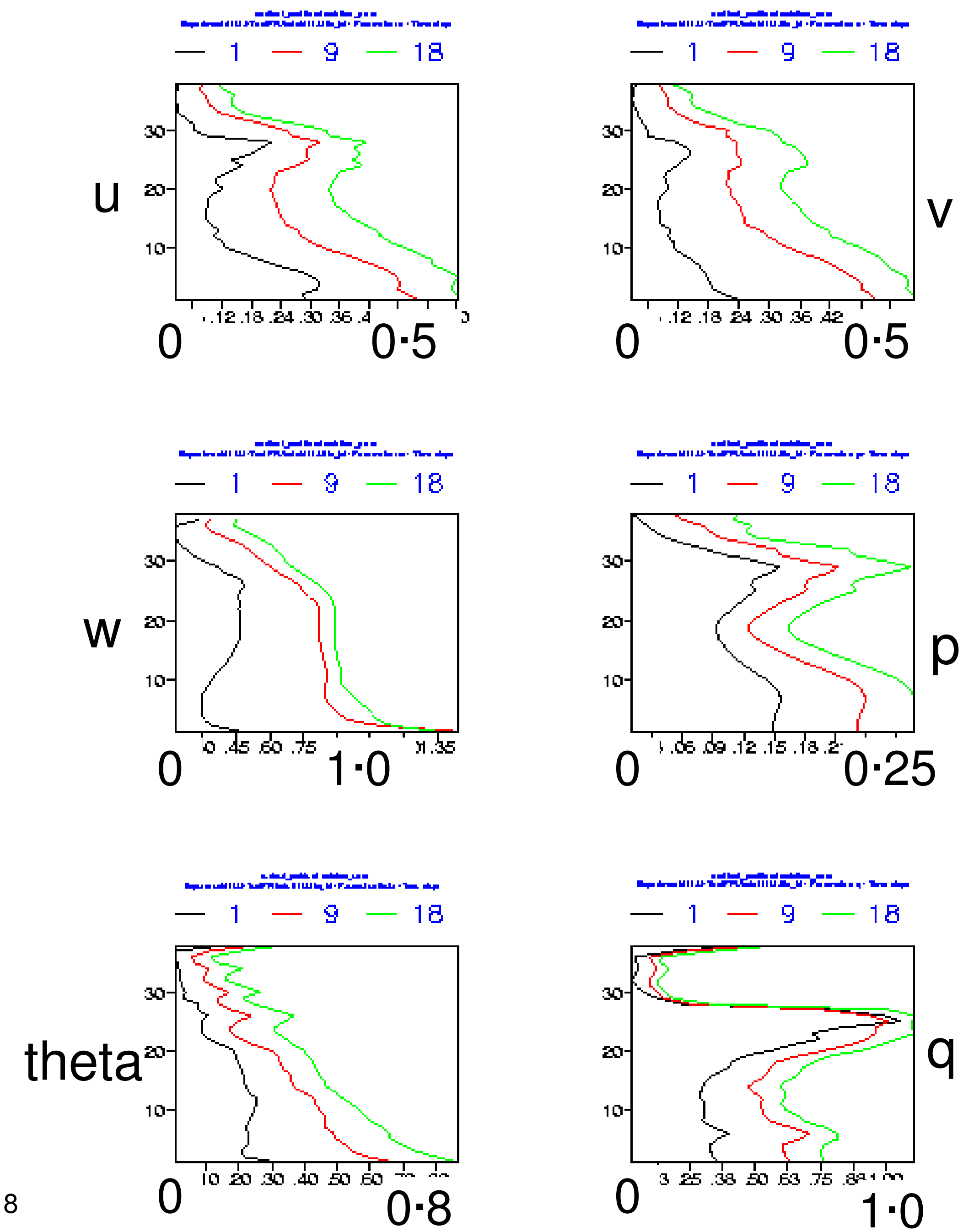
Evolution of solution error in PF model

(rms linearization error / rms non-linear increment)



Ballard et al (2006)

ECMWF Testing TL model in 4D-Var

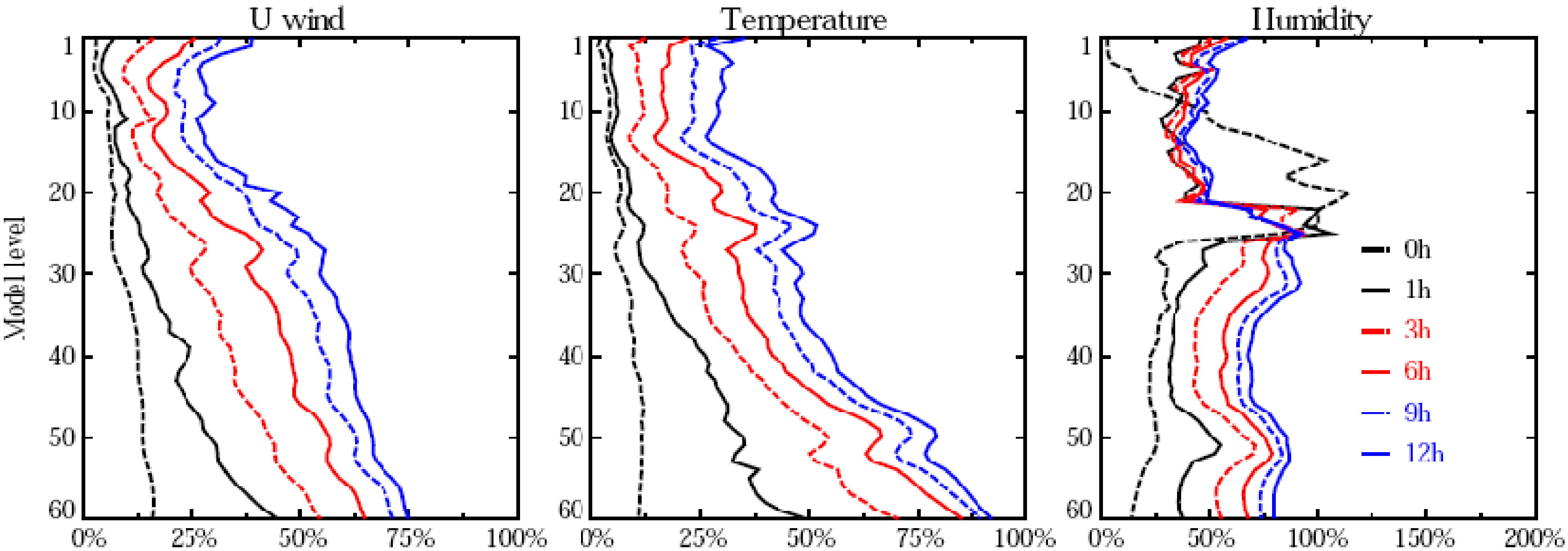


Figure 5: Evolution of the relative error in the T159 tangent linear model with respect to the T511 forecast model over the length of the assimilation window

Radnoti et al. (2005)

Benefit of outer-loop

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- The outer-loop is normally justified as a re-linearisation of a non-quadratic minimisation.

- It can also be thought of as a way of correcting for an imperfect Perturbation model, by reducing the amplitude of the perturbations whose trajectory is approximated:

$$\underline{\mathbf{y}} = \underline{\tilde{\mathbf{H}}}\underline{\tilde{\mathbf{M}}}\left(\delta\mathbf{x}, \underline{\boldsymbol{\eta}}\right) + \underline{\bar{H}}\left(\underline{\bar{M}}\left(\mathbf{x}^{g}, \underline{\boldsymbol{\eta}}^{g}\right)\right)$$

- Of course, with an imperfect perturbation model, there is no guarantee that an outer-loop will converge.

3. Developments in error modelling

Background error (prior) covariance **B** modelling assumptions

*The first operational 3D multivariate statistical analysis method (Lorenc 1981) made the following assumptions about the **B** which characterizes background errors,* ***all of which are wrong!***

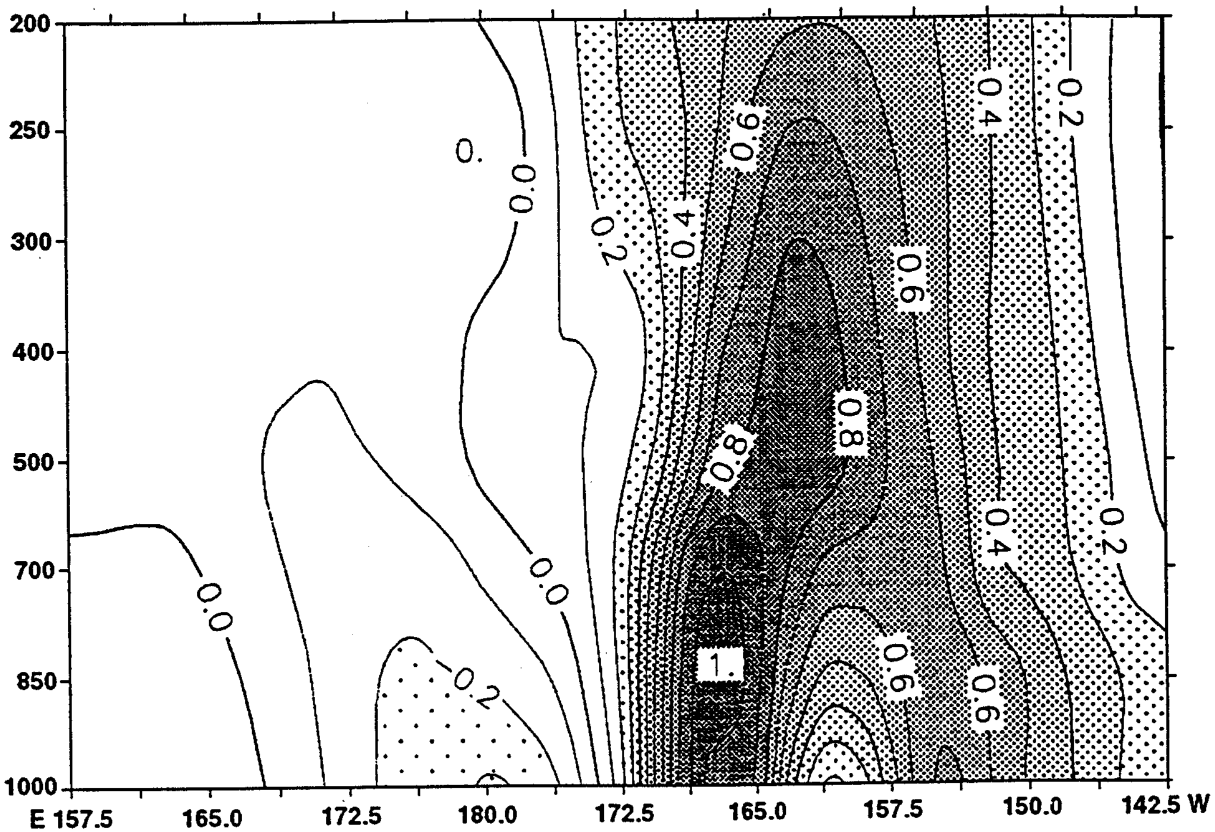
- Stationary – time & flow invariant
- Balanced – predefined multivariate relationships exist
- Homogeneous – same everywhere
- Isotropic – same in all directions
- 3D separable – horizontal correlation independent of vertical levels or structure & vice versa.

Since then many valiant attempts have been made to address them individually, but with limited success because of the errors remaining in the others. ***The most attractive ways of addressing them all are long-window 4D-Var or hybrid ensemble-VAR.***

3D Covariances dynamically generated by 4D-Var

If the time-period is long enough, the evolved 3D covariances also depend on the dynamics:

$$\mathbf{B}_{(x(t_n))} = \mathbf{M}_{n-1} \ldots \mathbf{M}_1 \mathbf{M}_0 \mathbf{B}_{(x(t_0))} \mathbf{M}_0^T \mathbf{M}_1^T \ldots \mathbf{M}_{n-1}^T$$



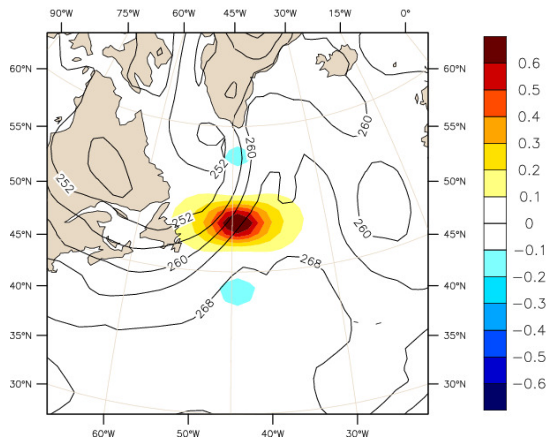
Cross-section of the 4D-Var structure function (using a 24 hour window).

Thépaut, Jean-Nöel, P. Courtier, G. Belaud and G Lemaître: 1996 "Dynamical structure functions in a four-dimensional variational assimilation: A case study" *Quart. J. Roy. Met. Soc.*, **122**, 535-561

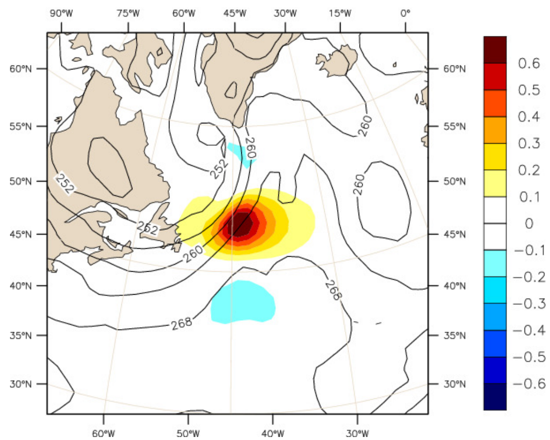
Single observation tests

u response to a single u observation at centre of window

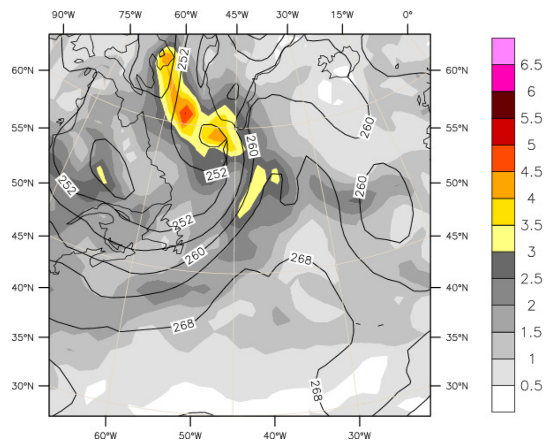
Horizontal



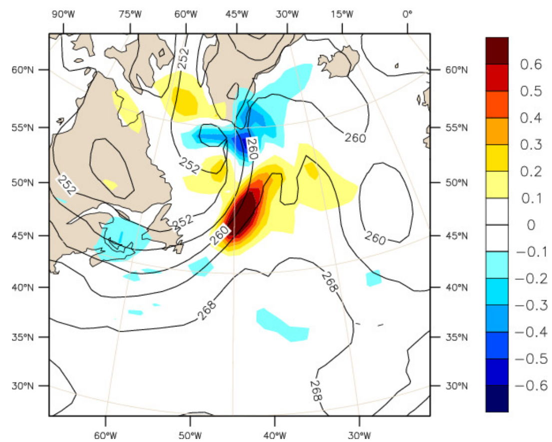
Standard 3D-Var



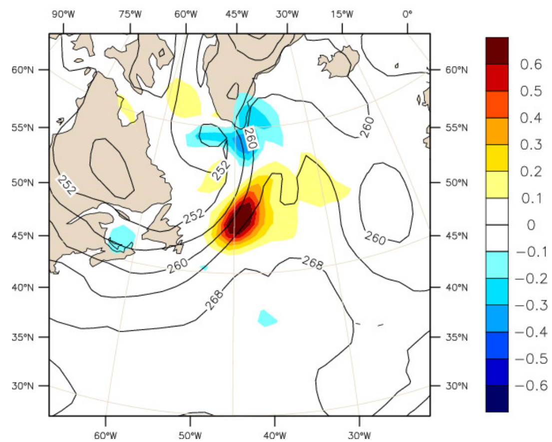
Standard 4D-Var



Ensemble RMS



Pure ensemble 3D-Var



50/50 hybrid 3D-Var

Adam Clayton

The nonlinear “Hólm” humidity transform

- Several centres have implemented a nonlinear humidity transform to compensate for the non-Gaussian errors of humidity forecasts (Hólm 2003, Gustafsson *et al.* 2011, Ingleby *et al.* in preparation)
- The “principle of symmetry” suggests a non-Gaussian prior:

$$P\left(RH \middle| RH^b\right) \propto \exp\left(\left(RH - RH^b\right)^2 \Big/ 2S\left[RH, RH^b\right]\right)$$

- This makes the variational minimisation implicit; ECMWF and HIRLAM iterate this term in the outer-loop, The Met Office include it in a non-quadratic inner minimisation.

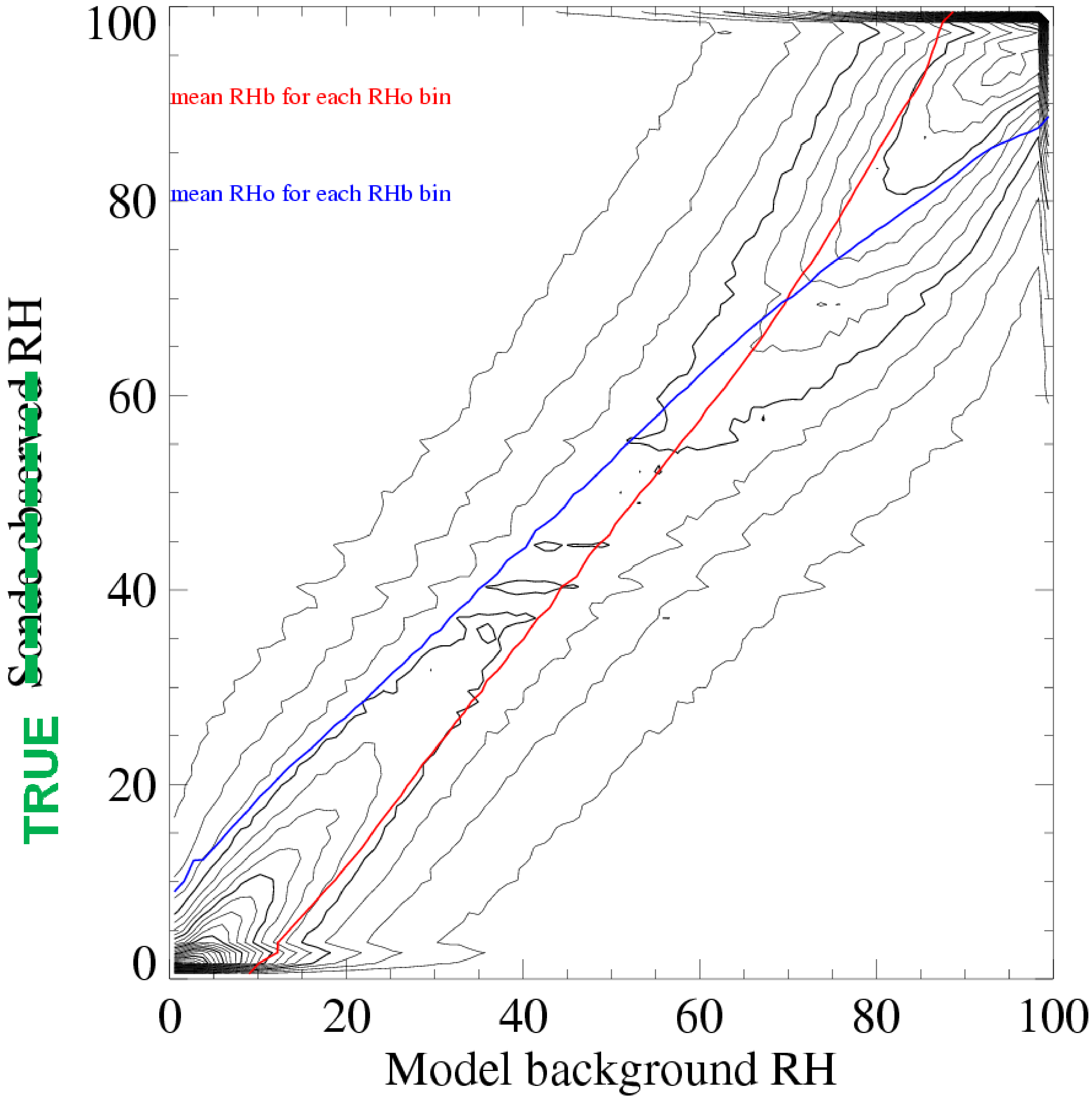
Effect of 0% & 100% limits on RH

$P(x \mid x^b)$ is biased, with mean given by blue line.

$\Rightarrow$ "best" estimate obtained by modifying x^b away from limits.

This would damage forecasts of cloud and rain!!

Diagram from Lorenc (2007)



Principle of symmetry and Hólm transform – a Bayesian interpretation.

What are the prior and loss function which make this optimal?

- The distribution of values in the background, generated by the model, is close to correct – we have the right cloud cover on average.
- It is important to us to retain this correct distribution – more so than to reduce the expected RMS error at each point.
- The Hólm transform constructs a (skewed) prior whose **mode** is the background.
- We rely on a minimisation which finds this **mode** (not the mean) and hence returns the model background unaltered in the absence of observations.

Fitting models of model error

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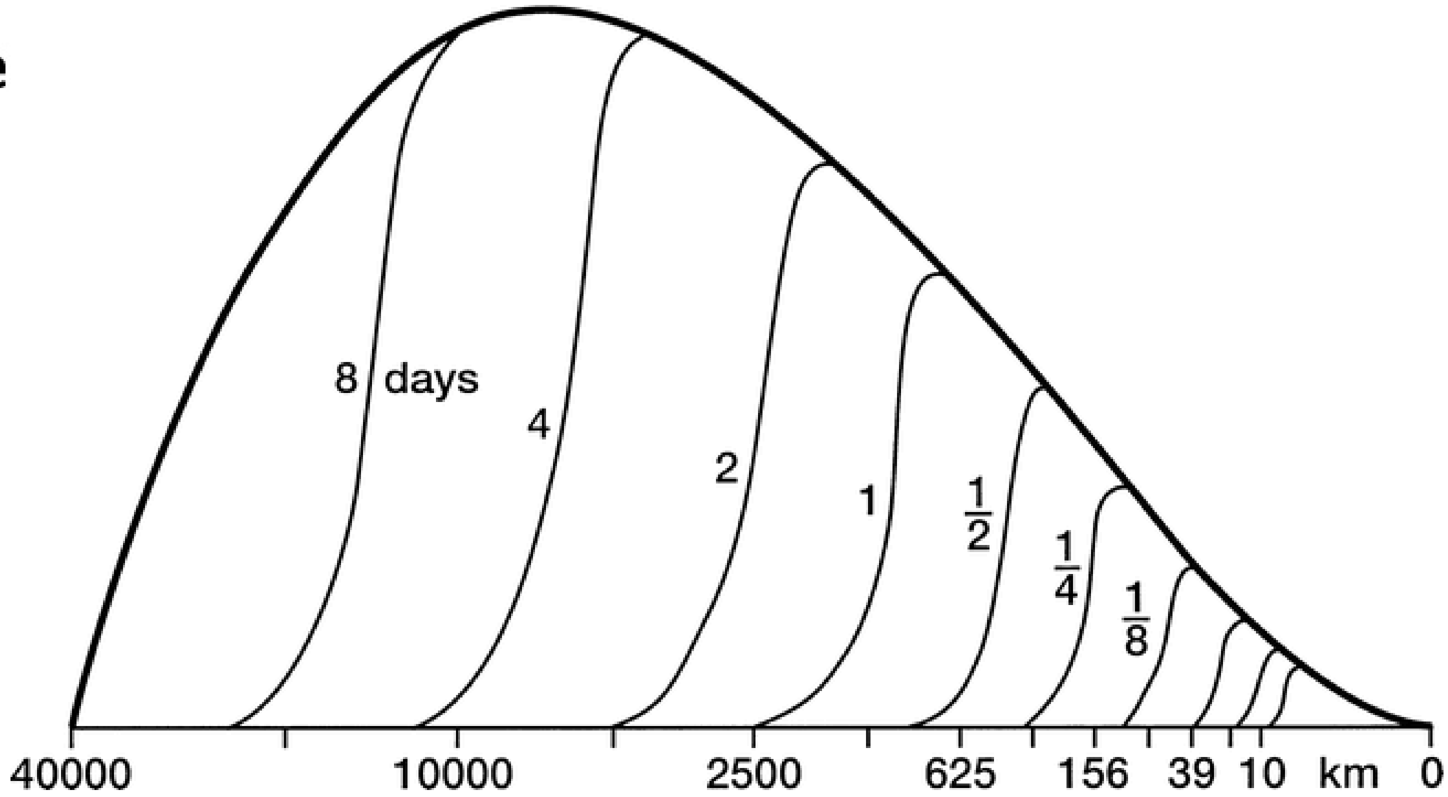
- The VAR approach encourages us to build ***physically based models of errors***: observational, representativity, background, observational bias, forecast model, … This approach is more likely to give a DA method applicable to a ***wide range of regimes***.

- We ***cannot uniquely fit*** these models to one set of o−b statistics. Nevertheless, as long as we have conceptual insight as to what should be common, we can use statistics from a range of regimes to estimate some of them (e.g. Hollingsworth and Lonnberg 1986, Desroziers *et al.* 2005, Dee 2005).

- Once we have a model of errors, we can augment the forecast model and determine uncertain coefficients in VAR. Tremolet (2007) has started applying these ideas to model error, but much remains to be done.

4. Coping with Butterflies

Error growth v scale



Growth of errors initially confined to smallest scales, according to a theoretical model Lorenz (1984) . Horizontal scales are on the bottom, and the upper curve is the full atmospheric motion spectrum. *(from Tribbia & Baumhefner 2004)*.

Long-window 4D-Var for a chaotic model

- Lorenc and Payne (2007) discussed 4D-Var for models with a ***wide range of scales*** – the small scales behave chaotically and cause problems. They suggested using a regularised linear model which filters poorly observed small scales (e.g. eddies in ocean DA, Hoteit *et al.* 2005).
- Abarbanel *et al.* (2010), approaching data assimilation as ***synchronised chaos***, say that there must be enough [observational] controls to move the positive conditional Lyapunov exponents on the synchronization manifold to negative values. (E.g. this was the case for the toy model used by Fisher *et al*. (2005)).
- Modern high-resolution global NWP models represent scales and regions (e.g. the middle atmosphere, Polavarapu *et al.* 2005) where neither approach is easy to apply.

Differences between identical NWP assimilations due to small initial perturbations.

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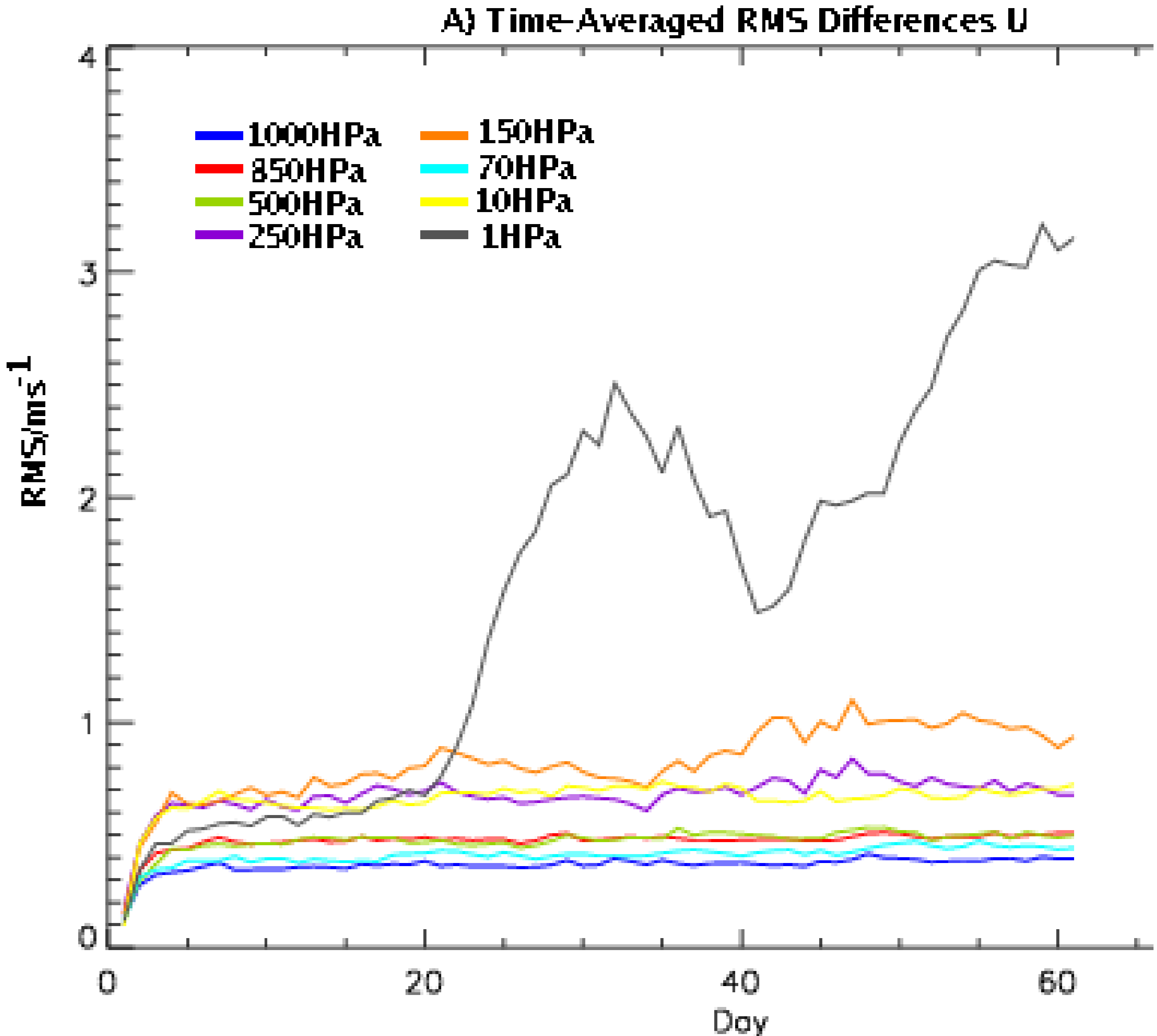
Global RMS differences between analysed u–fields at different levels.

Peter Jermey



Nonlinearity – benefitting from the attractor

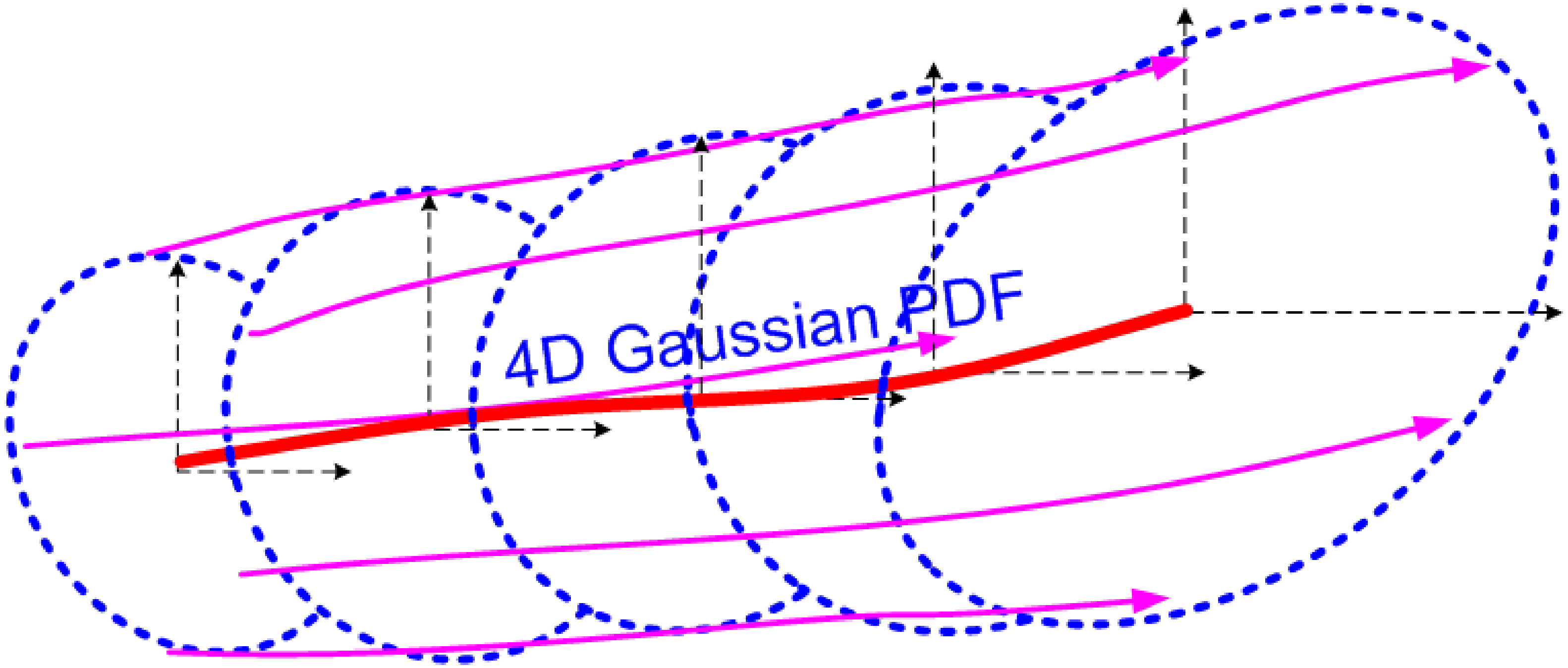
- The atmospheric state is fundamentally governed by nonlinear effects, e.g. convective-radiative equilibrium, condensation, cloud & precipitation. Nonlinear chaotic systems have a fuzzy ***attractor manifold*** of states that occur in reality – far fewer than all possible states. This gives us recognisable weather systems and practical weather prediction!
- Usual minimum variance **"best" estimate is not on the attractor**.
- The best practical way of defining the attractor in by using the full model, as we have for years in methods for ***spin-up*** and ***diabatic initialisation***.
- The VAR penalty function can only approximate near-linear aspects of this balance. We need to add an ***additional prior*** that we want the analysis to be a ***state which the model might generate***.
- Incremental VAR with an outer-loop can get us closer to this.

5. 4D-Ensemble-Var

Scalability – exploiting massively parallel computers

- 4D-Var as usually implemented 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, 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: ***4D–Ensemble-Var***. Other advantages of VAR can be retained.

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.

4D-En-Var - equations

Analysis variables are the localisation fields $\underline{\boldsymbol{\alpha}}_i$ multiplying each perturbation trajectory $\underline{\mathbf{x}}'_i$ to make the increment trajectory:

Lorenc (2003b), Liu *et al.* (2008), Buehner *et al.* (2010)

$$\delta\underline{\mathbf{x}} = \sum \underline{\boldsymbol{\alpha}}_i \circ \underline{\mathbf{x}}'_i$$

The increment trajectory plus the guess are interpolated to the obs:

$$\underline{\mathbf{y}} = \underline{\mathbf{H}}\delta\underline{\mathbf{x}} + \underline{H}\left(\underline{M}\left(\mathbf{x}^g, \underline{\boldsymbol{\eta}}^g\right)\right)$$

The penalty function is more akin to 3D-Var than 4D-Var:

We use standard transforms to model the spatial correlations in $\mathbf{C}$

$$J\left(\underline{\boldsymbol{\alpha}}\right) = \sum \tfrac{1}{2}\underline{\boldsymbol{\alpha}}_i^{\,T}\underline{\mathbf{C}}^{-1}\underline{\boldsymbol{\alpha}}_i + \tfrac{1}{2}\left(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o\right)^T \mathbf{R}^{-1}\left(\underline{\mathbf{y}} - \underline{\mathbf{y}}^o\right)$$

4D-En-Var. Outer-loop

$$\underline{\mathbf{y}} = \underline{\mathbf{H}}\delta\underline{\mathbf{x}} + \underline{H}\left(\underline{M}\left(\mathbf{x}^g, \underline{\boldsymbol{\eta}}^g\right)\right)$$

The analysis increment $\delta\underline{\mathbf{x}}$ may not be a model trajectory.

How best to add it to the full model to do outer-loop or to start the next DA cycle?

We want good fit to obs at end of window ***and*** a spun-up model.

Remember that the PF model is not an accurate approximation!

Invent a conceptual approximate PF model $\tilde{\underline{M}}$ such that

$$\delta\underline{\mathbf{x}} = \tilde{\underline{M}}\left(\delta\mathbf{x}, \underline{\boldsymbol{\eta}}\right)$$

Add $\delta\mathbf{x}$ to the background to give new $\mathbf{x}^g$ at the beginning of the window

and model error correction terms $\underline{\boldsymbol{\eta}}$ during forecast over window.

Conclusions

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1. Historical context

   Improvement from: high resolution, Bayes, advanced DA, better obs.
   4D-Var can fit a good model to high-res, indirect, incomplete obs.
   Complex NWP system needs modular development.

2. Reminder of 4D-Var derivations

   Fit deterministic model to obs v Bayesian best estimate.

3. Developments in error modelling

   Long window or ensemble best ways of improving all aspects.
   Non-Gaussian PDF should be symmetric in prior & posterior.

4. Coping with Butterflies

   Special treatment needed for important [unobserved] small scales.
   Use prior information that we want a state the model likes!

5. 4D-Ensemble-Var

   An attractive approach for future massively parallel computers.

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Questions and answers