

Introduction to data assimilation and least squares methods

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and many friends

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Contents

- Forecasting the weather - we are really getting better!
- Why: **Better obs?** **Better models?** **Better data assimilation?**
- Intro to data assim: a toy scalar example 1, **we measure with two thermometers**, and we want **an accurate temperature**.
- Another toy example 2, **we measure radiance** but we want **an accurate temperature**: we will derive **OI/KF**, **3D-Var**, **4D-Var** and **EnKF** for the toy model.
- The equations for the huge real systems are the same as for the toy models.

Some statistics of NWP...

Permanent verifications of the forecasts

ECMWF FORECAST VERIFICATION 12UTC

500hPa GEOPOTENTIAL

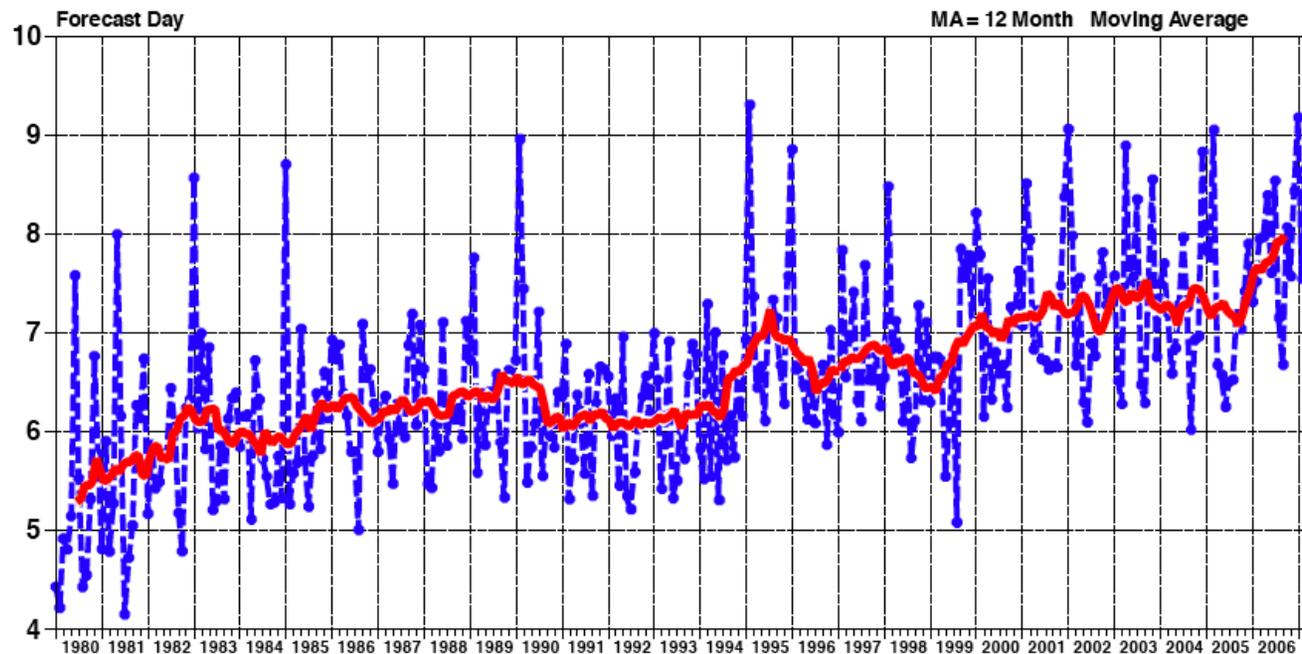
ANOMALY CORRELATION

FORECAST

EUROPE LAT 35.000 TO 75.000 LON -12.500 TO 42.500

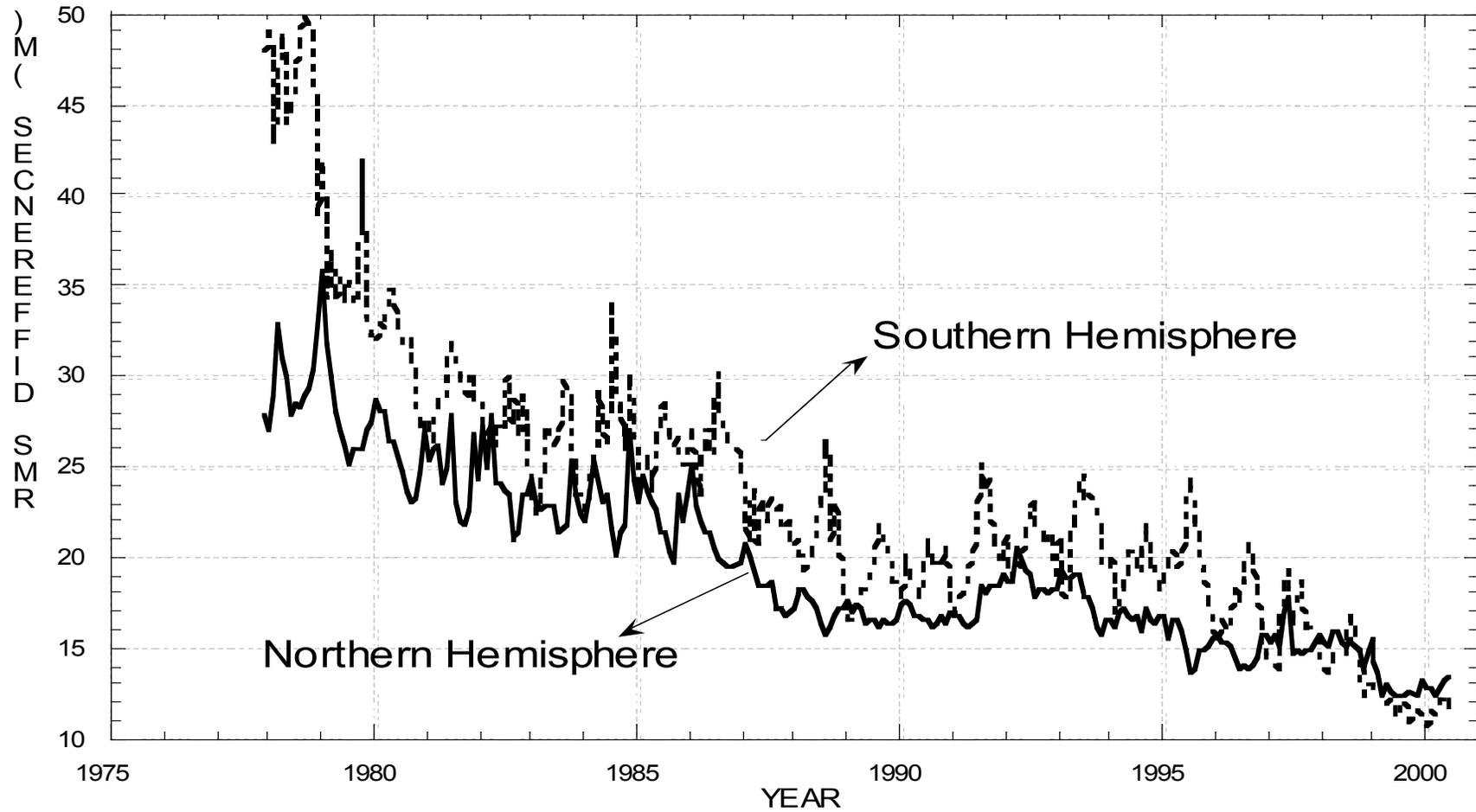
--- SCORE REACHES 60.00

— SCORE REACHES 60.00 MA



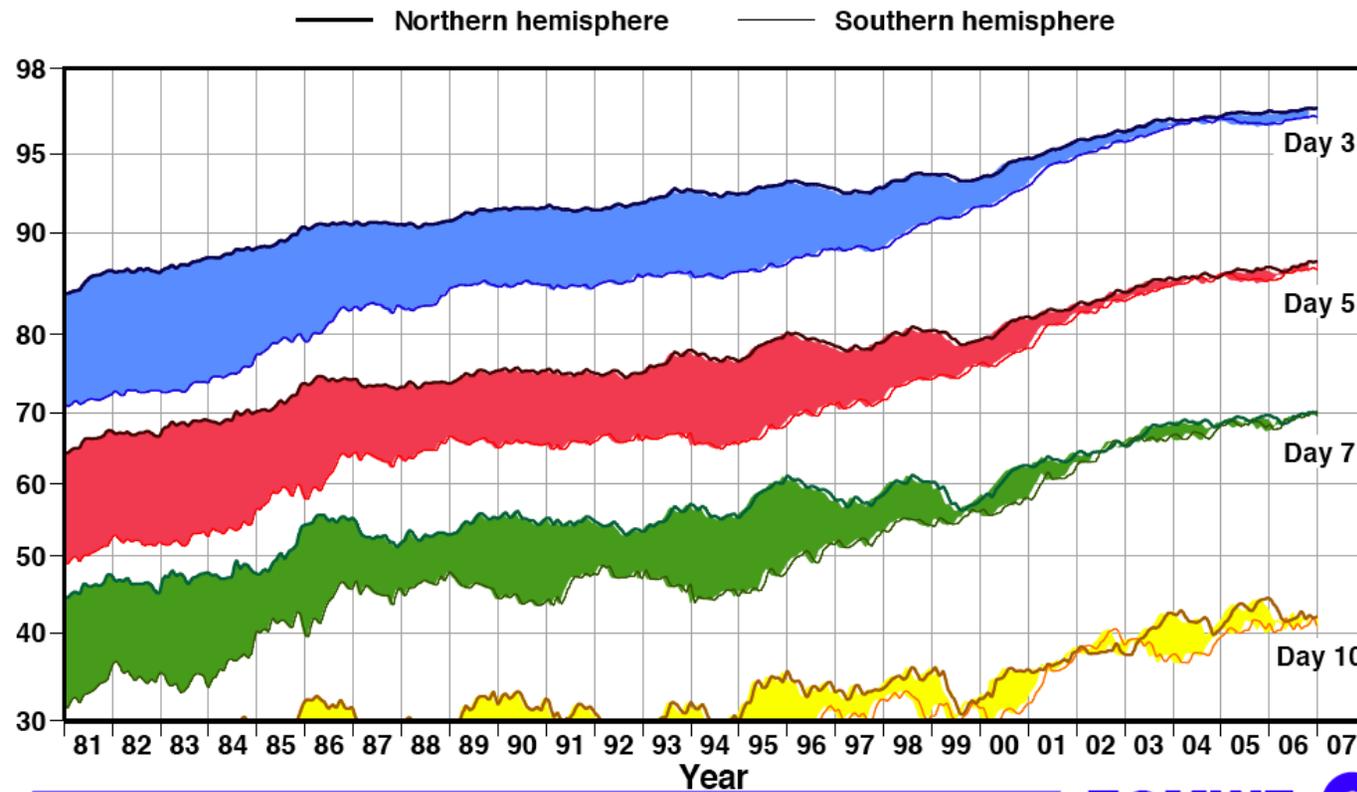
NCEP observational increments

500MB RMS FITS TO RAWINSONDES 6 HR FORECASTS



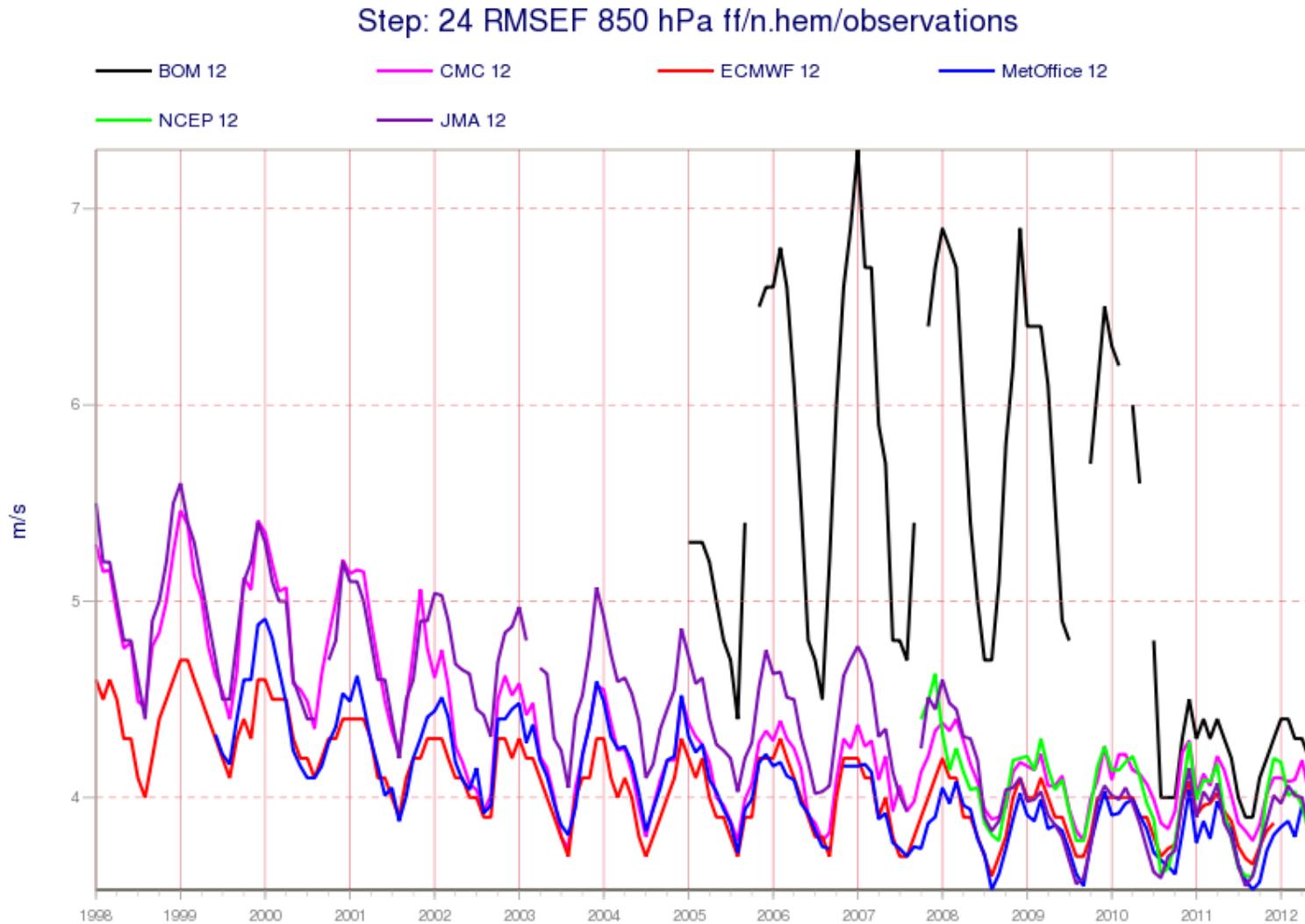
Comparisons of Northern and Southern Hemispheres

Anomaly correlation (%) of 500hPa height forecasts



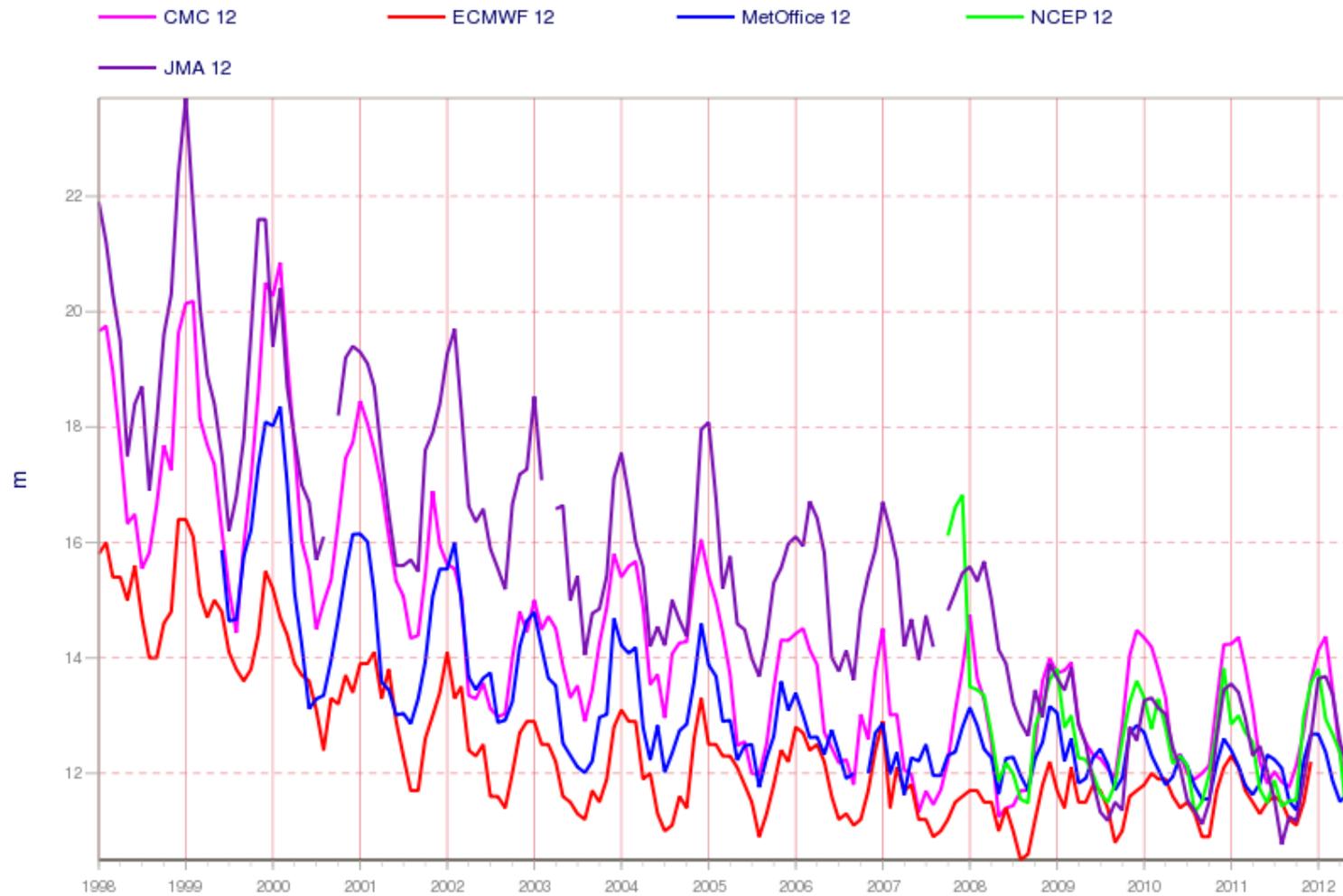
Comparisons verifying forecasts against observations

1-day forecasts, 850hPa, NH, verification of wind

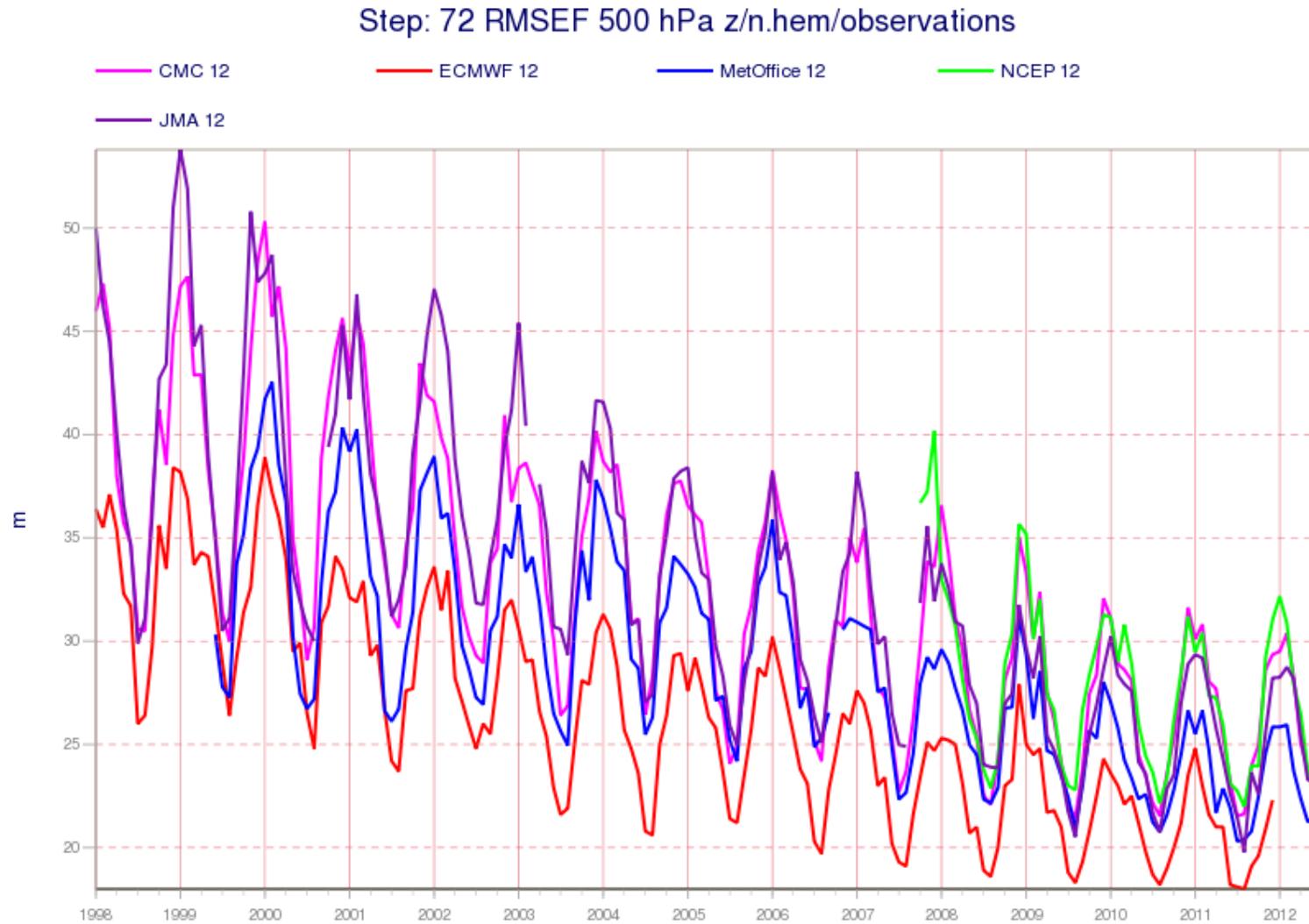


1-day forecast 500hPa Z, NH

Step: 24 RMSEF 500 hPa z/n.hem/observations

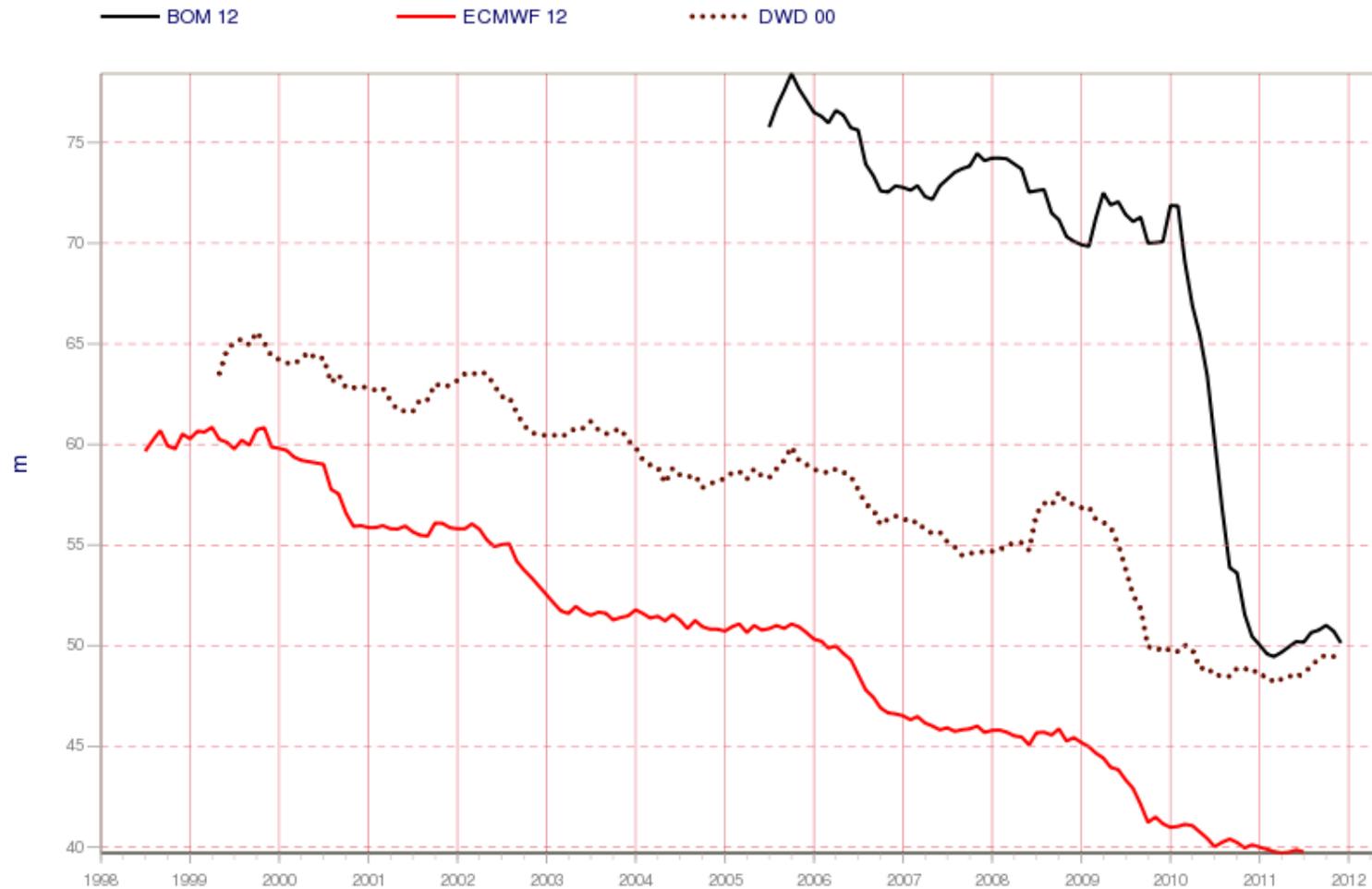


3-day forecast, 500hPa, NH against observations



5-day forecast, 500hPa, NH, 12 month average

Step: 120 RMSEF 500 hPa z/n.hem/observations



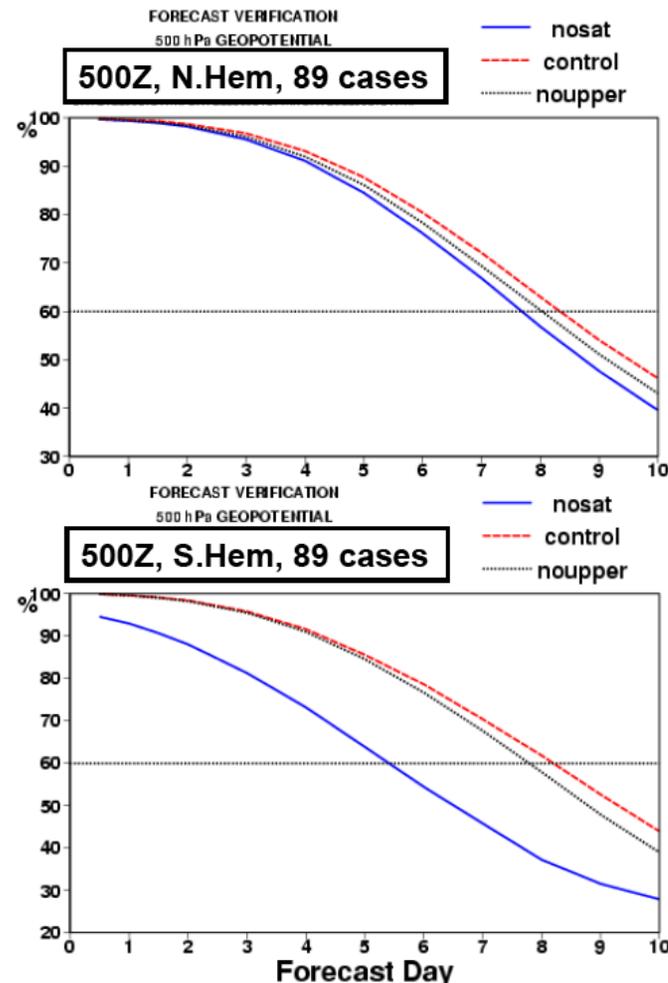
Satellite radiances are essential in the SH

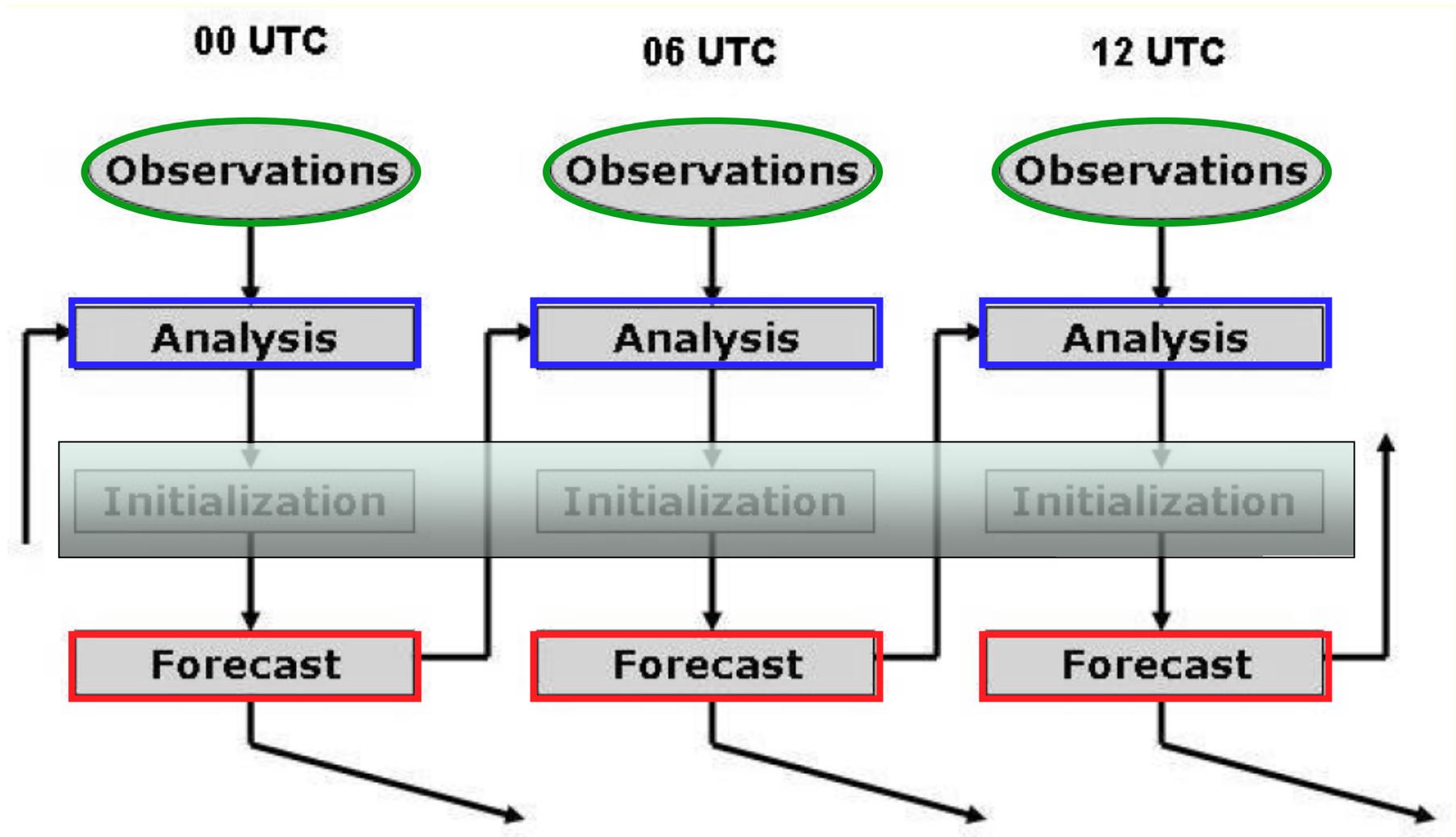
Observing System Experiments (ECMWF - G. Kelly et al.)

NoSAT= no satellite radiances or winds

Control= like operations

NoUpper=no radiosondes, no pilot winds, no wind profilers





Typical 6-hour analysis cycle.

Bayes interpretation: a forecast (the “prior”), is combined with the new observations, to create the Analysis (IC) (the “posterior”)

Intro. to data assim: toy example 1 summary

A **forecast** b and an **observation** o optimally combined (analysis):

$$T_a = T_b + \frac{\sigma_b^2}{\sigma_b^2 + \sigma_o^2} (T_o - T_b) \quad \text{with} \quad \frac{1}{\sigma_a^2} = \frac{1}{\sigma_b^2} + \frac{1}{\sigma_o^2}$$

***If** the statistics of the errors are exact, and if the coefficients are optimal, then the "precision" of the analysis (defined as the inverse of the variance) is the sum of the precisions of the measurements.*

Now we are going to see a second toy example of data assimilation including **remote sensing**.

The importance of these toy examples is that the equations are identical to those obtained with big models and many obs.

Intro. to remote sensing and data assimilation: toy example 2

- Assume we have an object, like a stone in space
- We want to estimate its temperature T (°K) accurately but we measure the radiance y (W/m²) that it emits. We have an *obs. model*, e.g.:

$$y = h(T) \sim \sigma T^4$$

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$$y = h(T) \sim \sigma T^4$$

- We also have a *forecast model* for the temperature

$$T(t_{i+1}) = m[T(t_i)];$$

$$\text{e.g., } T(t_{i+1}) = T(t_i) + \Delta t [\text{SW heating} + \text{LW cooling}]$$

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- We will derive the data assim eqs (KF and Var) for this toy system (easy to understand!)

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- We will derive the data assim eqs (OI/KF and Var) for this toy system (easy to understand!)
- Will compare the toy and the real huge vector/matrix equations: they are exactly the same!

Toy temperature data assimilation, measure radiance

We have a forecast T_b (prior) and a radiance obs $y_o = h(T_t) + \varepsilon_0$

The new information (or innovation) is the observational increment:

$$y_o - h(T_b)$$

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The final formula is very similar to that in toy model 1:

$$T_a = T_b + w(y_o - h(T_b))$$

with the optimal weight $w = \sigma_b^2 H (\sigma_o^2 + H \sigma_b^2 H)^{-1}$

Recall that $T_a = T_b + w(y_o - h(T_b)) = T_b + w(\varepsilon_o - H \varepsilon_b)$

So that, subtracting the truth, $\varepsilon_a = \varepsilon_b + w(\varepsilon_o - H \varepsilon_b)$

Toy temperature data assimilation, measure radiance

Summary for Optimal Interpolation/Kalman Filter (sequential):

$$T_a = T_b + w(y_o - h(T_b)) \quad \text{analysis}$$

with $w = \sigma_b^2 H (\sigma_o^2 + \sigma_b^2 H^2)^{-1}$ optimal weight

The analysis error is obtained from squaring $\varepsilon_a = \varepsilon_b + w[\varepsilon_o - H\varepsilon_b]$

$$\sigma_a^2 = \overline{\varepsilon_a^2} = (1 - wH)\sigma_b^2 = \frac{\sigma_o^2}{\sigma_o^2 + \sigma_b^2 H^2} \sigma_b^2$$

It can also be written as

$$\frac{1}{\sigma_a^2} = \left(\frac{1}{\sigma_b^2} + \frac{H^2}{\sigma_o^2} \right) \quad \begin{array}{l} \text{analysis precision=} \\ \text{forecast precision} + \text{observation precision} \end{array}$$

Toy temperature data assimilation, variational approach

We have a forecast T_b and a radiance obs $y_o = h(T_t) + \varepsilon_o$

Innovation: $y_o - h(T_b)$

From a 3D-Var point of view,
we want to find a T_a that
minimizes the cost function J :

$$J(T_a) = \frac{(T_a - T_b)^2}{2\sigma_b^2} + \frac{(h(T_a) - y_o)^2}{2\sigma_o^2}$$

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This analysis temperature T_a is closest to both the forecast T_b and the observation y_o and maximizes the likelihood of $T_a \sim T_{truth}$ given the information we have.

It is easier to find the analysis increment $T_a - T_b$ that minimizes the cost function J

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The cost function is derived from a maximum likelihood analysis:

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Likelihood of T_{truth} given T_b : $\frac{1}{\sqrt{2\pi}\sigma_b} \exp\left[-\frac{(T_{truth} - T_b)^2}{2\sigma_b^2}\right]$

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Toy temperature data assimilation, variational approach

We have a forecast T_b and a radiance obs $y_o = h(T_t) + \varepsilon_o$

Innovation: $y_o - h(T_b)$

From a 3D-Var point of view,
we want to find a T_a that
minimizes the cost function J :

$$2J_{\min} = \frac{(T_a - T_b)^2}{\sigma_b^2} + \frac{(h(T_a) - y_o)^2}{\sigma_o^2}$$

Likelihood of T_{truth} given T_b : $\frac{1}{\sqrt{2\pi}\sigma_b} \exp\left[-\frac{(T_{truth} - T_b)^2}{2\sigma_b^2}\right]$

Likelihood of $h(T_{truth})$ given y_o : $\frac{1}{\sqrt{2\pi}\sigma_o} \exp\left[-\frac{(h(T_{truth}) - y_o)^2}{2\sigma_o^2}\right]$

Joint likelihood of T_{truth} : $\frac{1}{\sqrt{2\pi}\sigma_b} \exp\left[-\frac{(T_{truth} - T_b)^2}{2\sigma_b^2} - \frac{(h(T_{truth}) - y_o)^2}{2\sigma_o^2}\right]$

Minimizing the cost function maximizes the likelihood of the estimate of truth

Toy temperature data assimilation, variational approach

Again, we have a forecast T_b and a radiance obs $y_o = h(T_t) + \varepsilon_0$

Innovation: $y_o - h(T_b)$

We want to find $(T_a - T_b)$ that minimizes the cost function J .

This maximizes the likelihood of

$T_a \sim T_{\text{truth}}$ given both T_b and y_o

$$2J_{\min} = \frac{(T_a - T_b)^2}{\sigma_b^2} + \frac{(h(T_a) - y_o)^2}{\sigma_o^2}$$

Toy temperature data assimilation, variational approach

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$$J(T_a) = \frac{(T_a - T_b)^2}{2\sigma_b^2} + \frac{(h(T_a) - y_o)^2}{2\sigma_o^2}$$

To find the minimum we use an incremental approach: find $T_a - T_b$:

$$h(T_a) - y_o = h(T_b) - y_o + H(T_a - T_b)$$

So that from $\partial J / \partial(T_a - T_b) = 0$ we get

$$(T_a - T_b) \left(\frac{1}{\sigma_b^2} + \frac{H^2}{\sigma_o^2} \right) = (T_a - T_b) \frac{1}{\sigma_a^2} = H \frac{(y_o - h(T_b))}{\sigma_o^2}$$

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or $T_a = T_b + w(y_o - h(T_b))$ where now

$$w = \left(\sigma_b^{-2} + H\sigma_o^{-2}H \right)^{-1} H\sigma_o^{-2} = \sigma_a^2 H\sigma_o^{-2}$$

Toy temperature data assimilation, variational approach

We have a forecast T_b and a radiance obs $y_o = h(T_t) + \varepsilon_o$

Innovation: $y_o - h(T_b)$

3D-Var: T_a minimizes the distance to both the background and the observations $2J_{\min} = \frac{(T_a - T_b)^2}{\sigma_b^2} + \frac{(h(T_a) - y_o)^2}{\sigma_o^2}$

3D-Var solution $T_a = T_b + w(y_o - h(T_b))$ with $w = (\sigma_b^{-2} + H\sigma_o^{-2}H)^{-1} H\sigma_o^{-2} = \sigma_a^2 H\sigma_o^{-2}$

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This variational solution is the same as the one obtained before with Kalman filter (a sequential approach, like Optimal Interpolation, Lorenc 86):

KF/OI solution $T_a = T_b + w(y_o - h(T_b))$ with $w_{OI} = \sigma_b^2 H (\sigma_o^2 + \sigma_b^2 H^2)^{-1}$

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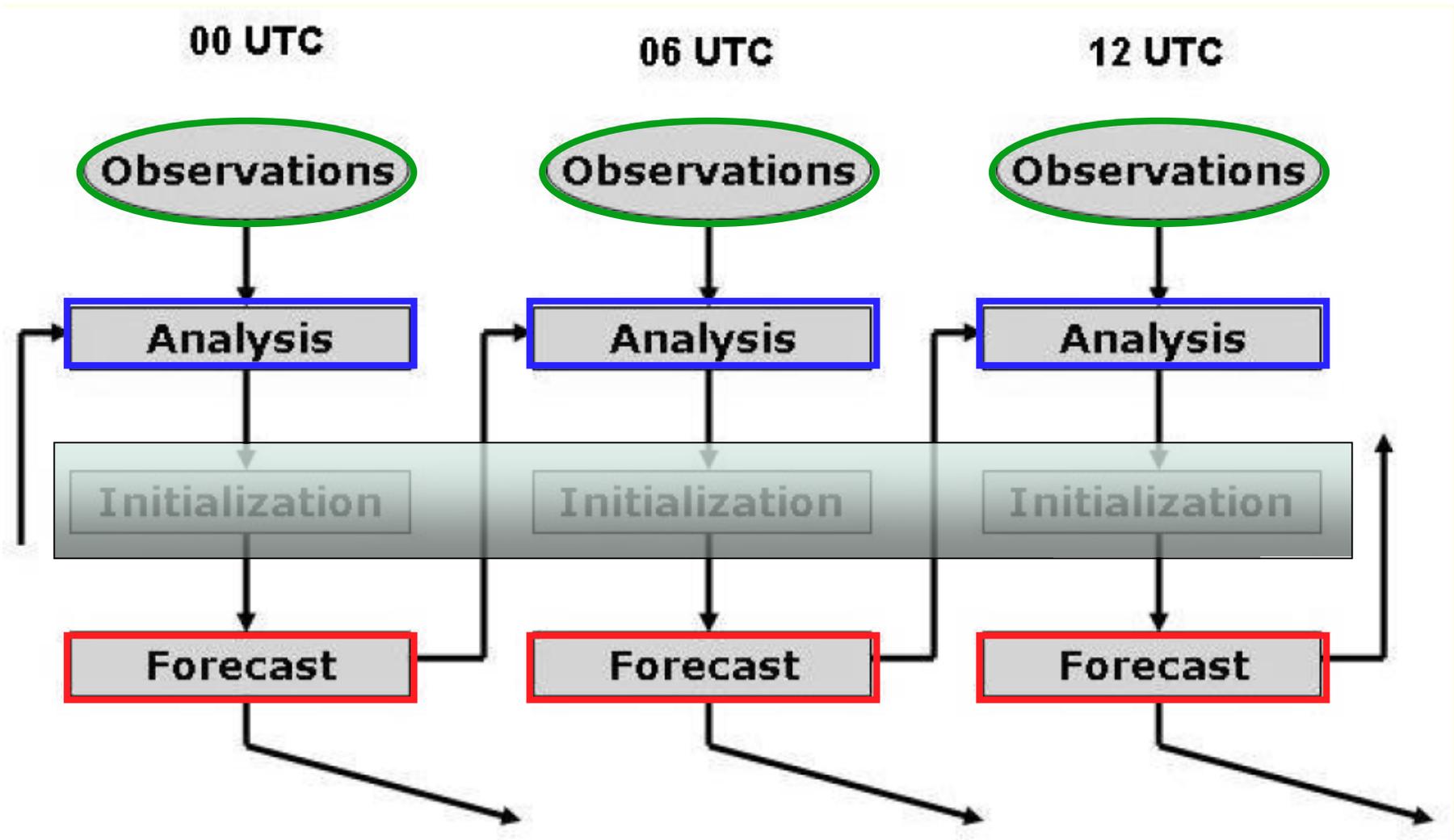
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Show that the 3d-Var and the OI/KF weights are the same: both methods find the same optimal solution!



Typical 6-hour analysis cycle.

Forecast phase, followed by Analysis phase

Toy temperature **analysis cycle** (Kalman Filter)

Forecasting phase, from t_i to t_{i+1} : $T_b(t_{i+1}) = m[T_a(t_i)]$

Forecast error: $\varepsilon_b(t_{i+1}) = T_b(t_{i+1}) - T_t(t_{i+1}) =$
 $m[T_a(t_i)] - m[T_t(t_i)] + \varepsilon_m(t_{i+1}) = M\varepsilon_a(t_i) + \varepsilon_m(t_{i+1})$

So that we can predict the forecast error variance

$$\sigma_b^2(t_{i+1}) = M^2 \sigma_a^2(t_i) + Q_i; \quad Q_i = \overline{\varepsilon_m^2(t_{i+1})}$$

(The forecast error variance comes from the **analysis** and **model errors**)

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(The forecast error variance comes from the **analysis** and **model errors**)

Now we can compute the optimal weight (**KF** or **Var**, whichever form is more convenient, since they are equivalent):

$$w = \sigma_b^2 H (\sigma_o^2 + H \sigma_b^2 H)^{-1} = \left(\sigma_b^{-2} + H \sigma_o^{-2} H \right)^{-1} H \sigma_o^{-2}$$

Toy temperature analysis cycle (Kalman Filter)

Analysis phase: we use the new observation $y_o(t_{i+1})$

compute the new observational increment $y_o(t_{i+1}) - h(T_b(t_{i+1}))$

and the new analysis:

$$T_a(t_{i+1}) = T_b(t_{i+1}) + w_{i+1} \left[y_o(t_{i+1}) - h(T_b(t_{i+1})) \right]$$

We also need to compute the new analysis error variance:

$$\text{from } \sigma_a^{-2} = \sigma_b^{-2} + H \sigma_o^{-2} H$$

$$\text{we get } \sigma_a^2(t_{i+1}) = \left(\frac{\sigma_o^2 \sigma_b^2}{\sigma_o^2 + H^2 \sigma_b^2} \right)_{i+1} = (1 - w_{i+1} H) \sigma_{b_{i+1}}^2 < \sigma_{b_{i+1}}^2$$

now we can advance to the next cycle t_{i+2}, t_{i+3}, \dots

Summary of toy Analysis Cycle (for a scalar)

$$T_b(t_{i+1}) = m[T_a(t_i)] \quad \sigma_b^2(t_{i+1}) = M^2[\sigma_a^2(t_i)] \quad M = \partial m / \partial T$$

Interpretation...

“We use the model to forecast T_b and to update the forecast error variance from t_i to t_{i+1} ”

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“We use the model to forecast T_b and to update the forecast error variance from t_i to t_{i+1} ”

$$\text{At } t_{i+1} \quad T_a = T_b + w[y_o - h(T_b)]$$

“The analysis is obtained by adding to the background the innovation (difference between the observation and the first guess) multiplied by the optimal weight:

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$$w = \sigma_b^2 H (\sigma_o^2 + H \sigma_b^2 H)^{-1}$$

“The optimal weight is the background error variance divided by the sum of the observation and the background error variance. $H = \partial h / \partial T$ ensures that the magnitudes and units are correct.”

Summary of toy Analysis Cycle (for a scalar)

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“The optimal weight is the background error variance divided by the sum of the observation and the background error variance. $H = \partial h / \partial T$ ensures that the magnitudes and units are correct.”

Note that the larger the background error variance, the larger the correction to the first guess.

Summary of toy Analysis Cycle (for a scalar)

The analysis error variance is given by

$$\sigma_a^2 = \left(\frac{\sigma_o^2 \sigma_b^2}{\sigma_o^2 + H^2 \sigma_b^2} \right) = (1 - wH) \sigma_b^2$$

“The analysis error variance is reduced from the background error by a factor (1 - scaled optimal weight)”

Summary of toy system equations (cont.)

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“The analysis error variance is reduced from the background error by a factor (1 - scaled optimal weight)”

This can also be written as

$$\sigma_a^{-2} = \left(\sigma_b^{-2} + \sigma_o^{-2} H^2 \right)$$

“The analysis precision is given by the sum of the background and observation precisions”

Equations for toy and real **huge** systems

These statements are important because they hold true for data assimilation systems in **very** large multidimensional problems (e.g., NWP).

Instead of model, analysis and observational scalars, we have 3-dimensional vectors of sizes of the order of 10^7 - 10^9

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Instead of model, analysis and observational scalars, we have 3-dimensional vectors of sizes of the order of 10^7 - 10^8

We have to replace scalars (obs, forecasts) by vectors

$$T_b \rightarrow \mathbf{x}_b; \quad T_a \rightarrow \mathbf{x}_a; \quad y_o \rightarrow \mathbf{y}_o;$$

and their error variances by error covariances:

$$\sigma_b^2 \rightarrow \mathbf{B}; \quad \sigma_a^2 \rightarrow \mathbf{A}; \quad \sigma_o^2 \rightarrow \mathbf{R};$$

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Interpretation of the NWP system of equations

“We use the model to forecast from t_i to t_{i+1} ”

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At t_{i+1} $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}[\mathbf{y}_o - H(\mathbf{x}_b)]$

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“The analysis is obtained by adding to the background the innovation (difference between the observation and the first guess) multiplied by the optimal Kalman gain (weight) matrix”

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“The optimal weight is the background error covariance divided by the sum of the observation and the background error covariance.

$\mathbf{H} = \partial H / \partial \mathbf{x}$ ensures that the magnitudes and units are correct.

The larger the background error variance, the larger the correction to the first guess.”

Interpretation of the NWP system of equations

Forecast phase:

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“We use the linear tangent model and its adjoint to forecast **B**”

$$\mathbf{B}(t_{i+1}) = \mathbf{M}[\mathbf{A}(t_i)]\mathbf{M}^T$$

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“However, this step is so horrendously expensive that it makes Kalman Filter completely unfeasible”.

“Ensemble Kalman Filter solves this problem by estimating **B** using an ensemble of forecasts.”

Summary of NWP equations (cont.)

The analysis error covariance is given by

$$\mathbf{A} = (\mathbf{I} - \mathbf{KH})\mathbf{B}$$

“The analysis covariance is reduced from the background covariance by a factor ($\mathbf{I} -$ scaled optimal gain)”

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“The analysis precision is given by the sum of the background and observation precisions”

$$\mathbf{K} = \mathbf{B}\mathbf{H}^T (\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1} = (\mathbf{B}^{-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H})^{-1} \mathbf{H}^T \mathbf{R}^{-1}$$

“The **variational** approach and the **sequential** approach are solving the same problem, with the same \mathbf{K} , but only KF (or EnKF) provide an estimate of the analysis error covariance”

Ensemble Transform Kalman Filter (EnKF)

Forecast step:

$$\mathbf{x}_{n,k}^b = M_n \left(\mathbf{x}_{n-1,k}^a \right)$$
$$\mathbf{B}_n = \frac{1}{K-1} \mathbf{X}_n^b \mathbf{X}_n^{bT}, \text{ where } \mathbf{X}_n^b = \left[\mathbf{x}_{n,1}^b - \bar{\mathbf{x}}_n^b; \dots, \mathbf{x}_{n,K}^b - \bar{\mathbf{x}}_n^b \right]$$

Analysis step:

$$\mathbf{x}_n^a = \mathbf{x}_n^b + \mathbf{K}_n (\mathbf{y}_n - H\bar{\mathbf{x}}_n^b); \mathbf{K}_n = \mathbf{B}_n \mathbf{H}^T (\mathbf{R} + \mathbf{H}\mathbf{B}_n \mathbf{H}^T)^{-1}$$

The new analysis error covariance in the ensemble space is (Hunt et al. 2007)

$$\tilde{\mathbf{A}}_n = \left[(K-1)\mathbf{I} + (\mathbf{H}\mathbf{X}_n^b)^T \mathbf{R}^{-1} (\mathbf{H}\mathbf{X}_n^b) \right]^{-1}$$

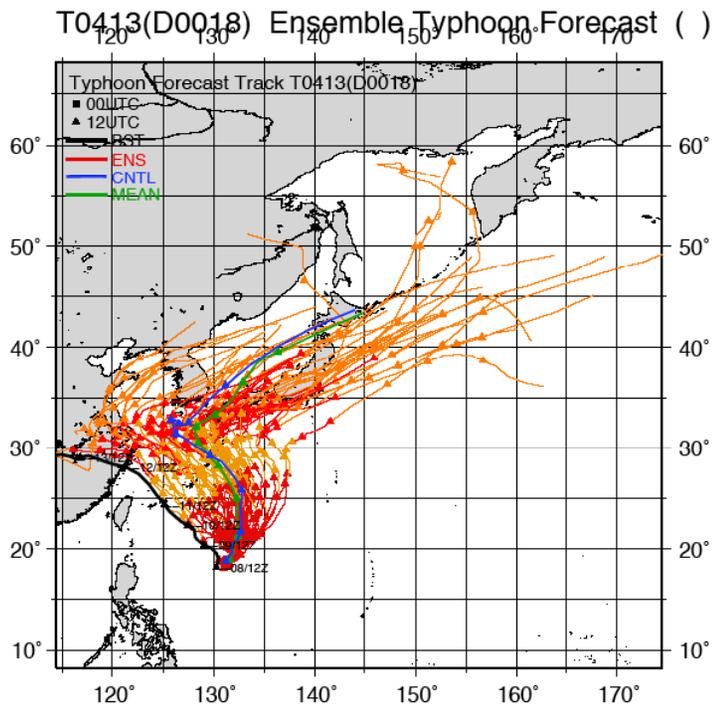
And the new ensemble perturbations are given by (transform)

$$\mathbf{X}_n^a = \mathbf{X}_n^b \left[(K-1)\tilde{\mathbf{A}}_n \right]^{1/2}$$

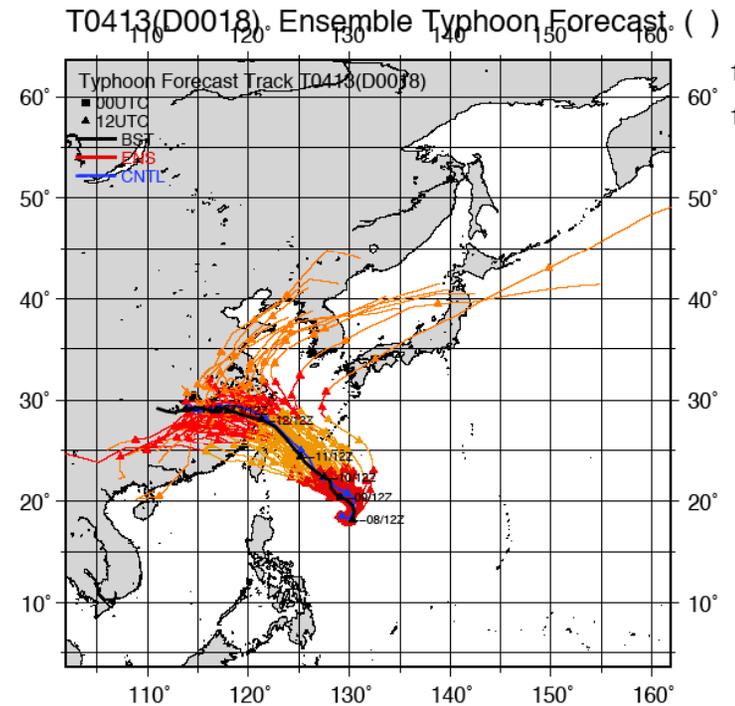
Comparison of 4-D Var and LETKF at JMA

18th typhoon in 2004, IC 12Z 8 August 2004

T. Miyoshi and Y. Sato

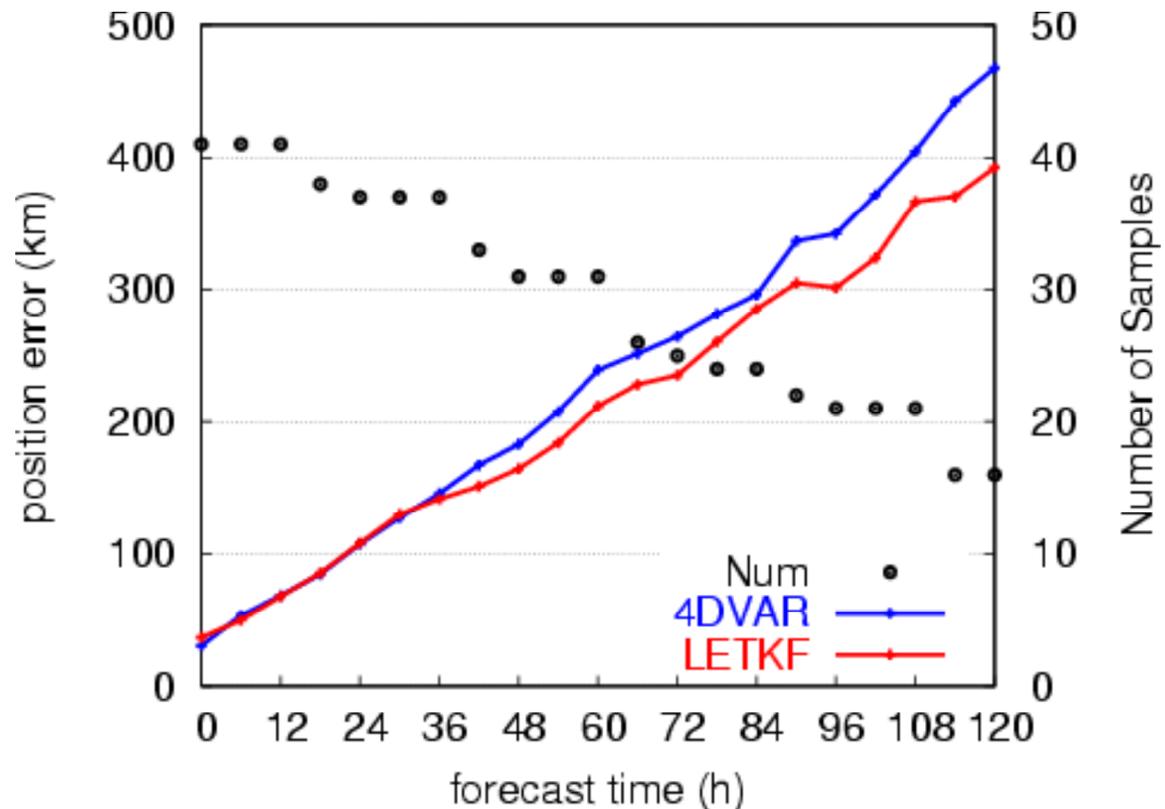


operational



LETKF

Comparison of 4-D Var and LETKF at JMA
RMS error statistics for all typhoons in August 2004
T. Miyoshi and Y. Sato



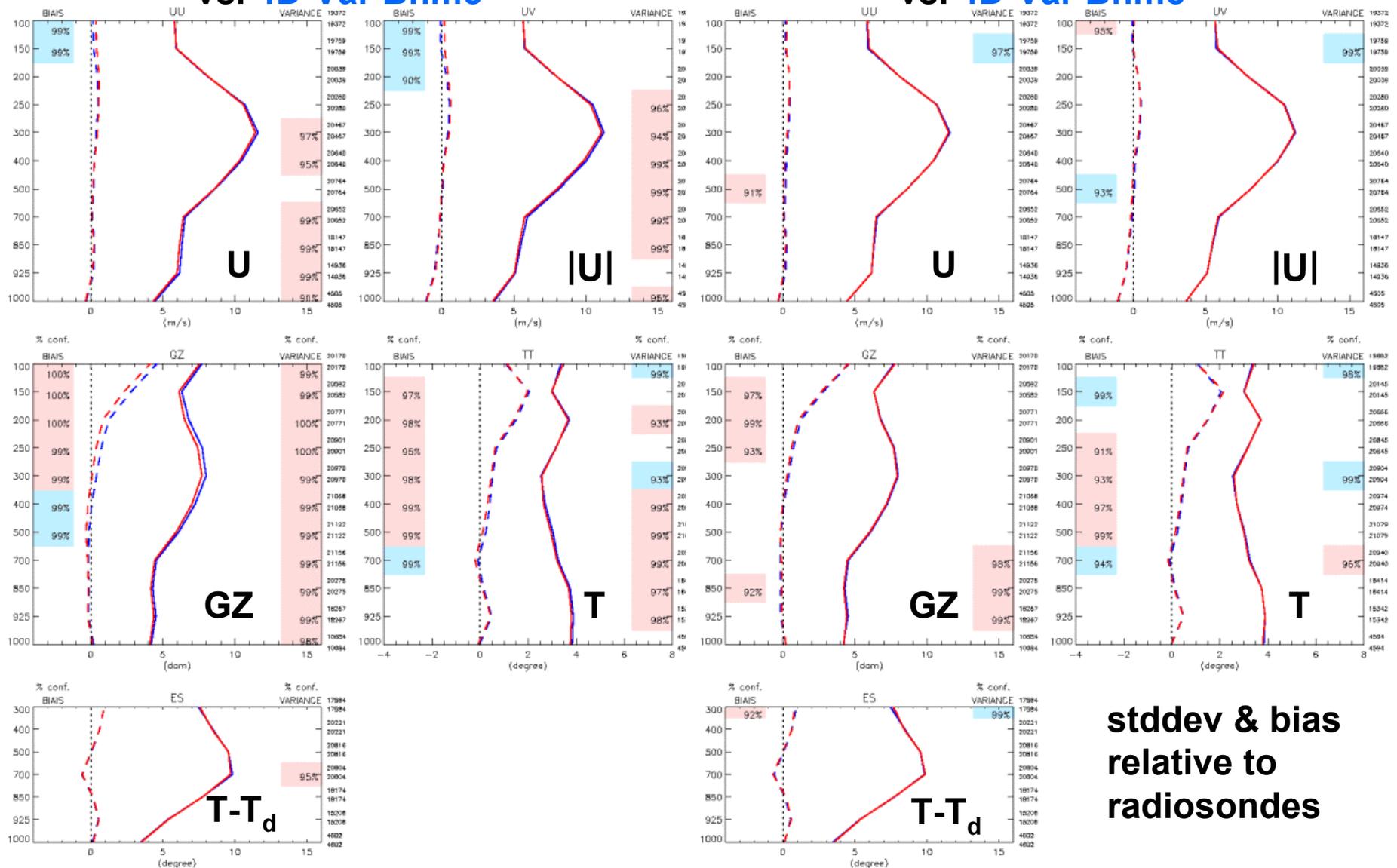
Operational 4D-Var

LETKF

Buehner et al., 2008: Forecast Results – 120h NH

EnKF mean analysis
vs. 4D-Var Bnmc

4D-Var Benkf
vs. 4D-Var Bnmc **HYBRID**

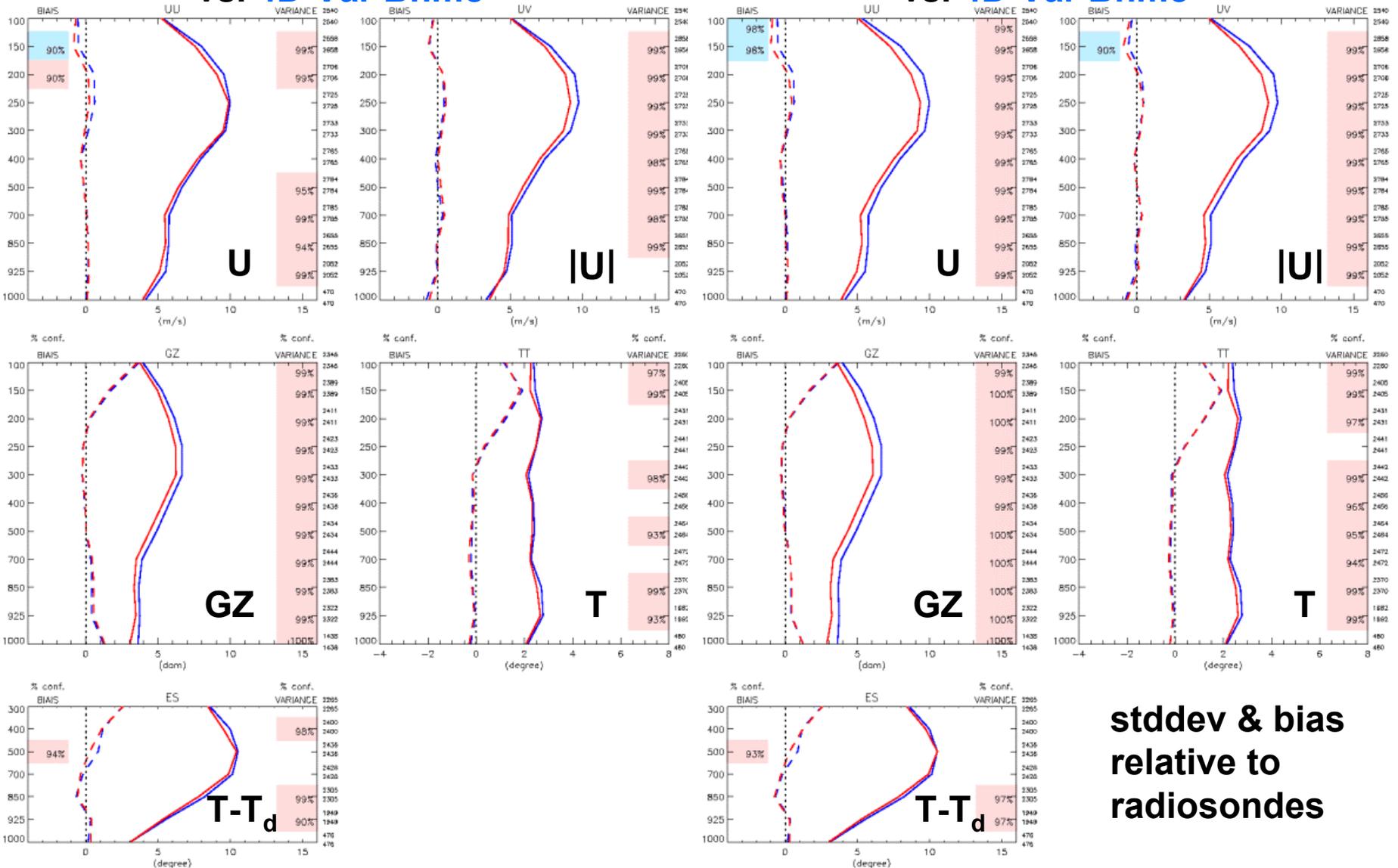


stddev & bias
relative to
radiosondes

Buehner et al., 2008: Forecast Results – 120h SH

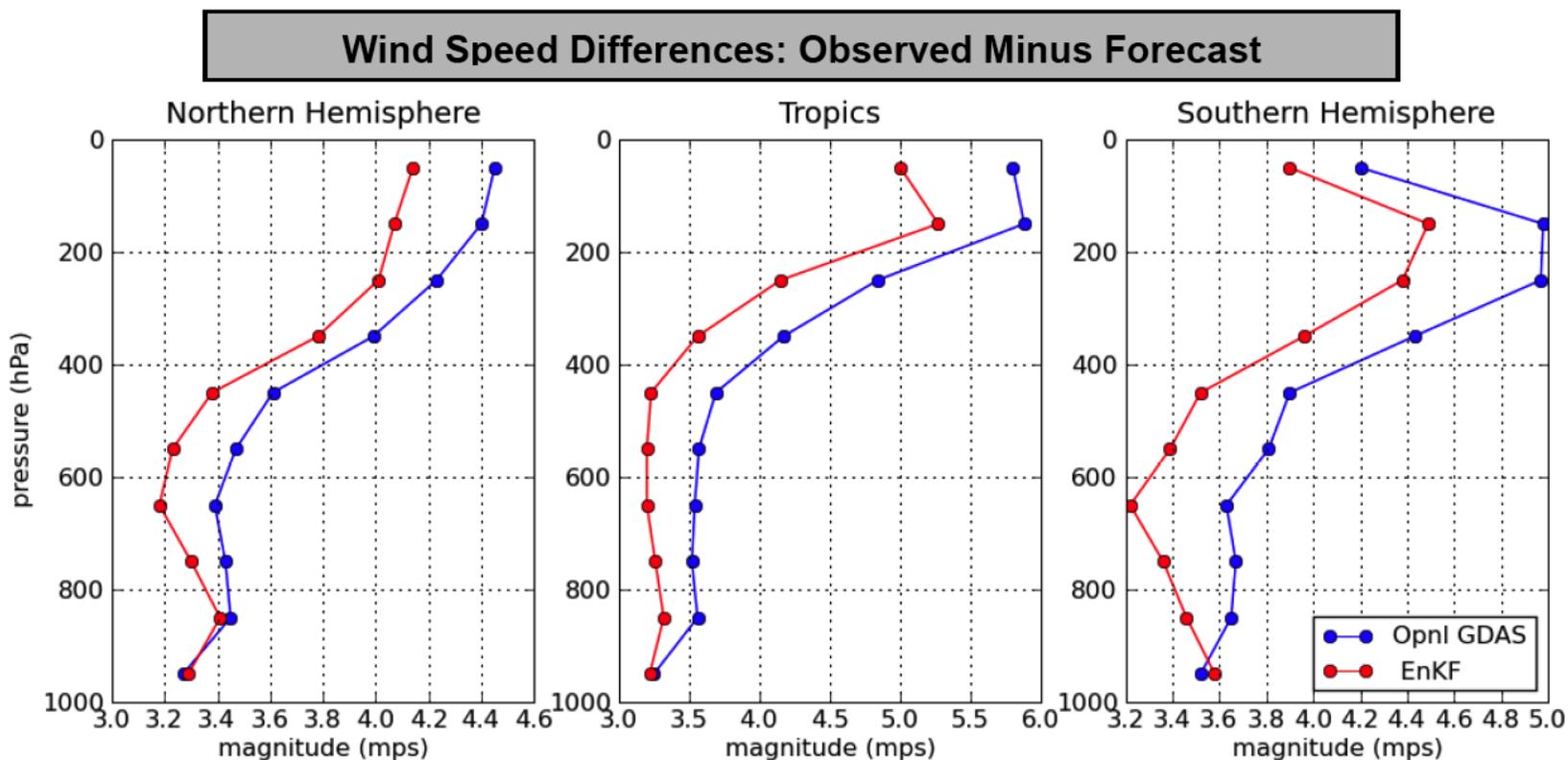
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Whitaker: Comparison of T190, 64 members EnKF with T382 operational GSI, same observations



Vertical profiles of the RMS difference between six hour forecasts and in-situ observations for the period 2007120700 – 2008010718. Observations are aggregated in 100 hPa layers. The red curve is for the ensemble mean of the experimental 64-member T190 EnKF system, and the blue curve is for the T382 GSI-based GDAS system operational in December 2007.

Summary

- Data assimilation methods have contributed much to the improvements in NWP.
- A toy example is easy to understand, and the equations are the same for a realistic system
- Kalman Filter (too costly) and 4D-Var (complicated) solve the same problem if the model is linear and we use long assimilation windows
- Ensemble Kalman Filter is feasible and simple, and is starting to catch up with operational 4D-Var (hybrid).
- **Important problems:** estimate and correct model errors & obs. errors, optimal obs. types and locations, tuning additive/multiplicative inflation, parameters estimation,...
- It seems like EnKF data assimilation could be used for parameter estimation and hence for model correction.
- I'll show new applications for EnKF in the 2nd talk